Supporting information for:

16OSTM10: A new open-shell transition metal conformational energies database to challenge contemporary semiempirical and force field methods

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Contents:

Tables forming the basis of Figures 2-8 in the main text....3
Table S1. Table forming the basis of Figure 2....3
Table S2. Table forming the basis of Figure 3....3
Table S3. Table forming the basis of Figure 4....5
Table S4. Table forming the basis of Figure 5....6
Table S5. Table forming the basis of Figure 6....9
Table S6. Table forming the basis of Figure 7....9
Table S7. Table forming the basis of Figure 8....10
Table S8. T1/T2 diagnostic values for 10 compounds of 16OSTM10 database....14
FOD plots....14
Figure S1. Qualitative FOD diagnostics for FIYMEI. The isosurface value is σ = 0.005 e/Bohr^3. 14
Figure S2. Qualitative FOD diagnostics for UZEYAA. The isosurface value is σ = 0.005 e/Bohr^3. 15
Figure S3. Qualitative FOD diagnostics for FUDNIB. The isosurface value is σ = 0.005 e/Bohr^3. 16
Figure S4. Qualitative FOD diagnostics for YIKLUC. The isosurface value is σ = 0.005 e/Bohr^3. 16
Figure S5. Qualitative FOD diagnostics for AJOMIX. The isosurface value is σ = 0.005 e/Bohr^3. 17
Figure S6. Qualitative FOD diagnostics for LIBLEN. The isosurface value is σ = 0.005 e/Bohr^3. 17
Composition of the λ1 and λ2 basis sets used in the Priroda calculations....17
Tabulated absolute conformational energies and optimized Cartesian coordinates for the compounds of 16OSTM10 database. 18

Tables forming the basis of Figures 2-8 in the main text

Table S1. Table forming the basis of Figure 2.

Method	PBE	PBE0	M06	ωB97X-V
min	0.42	0.68	0.65	0.36
average	0.91	0.94	0.92	0.87
max	0.99	1.00	0.99	0.99
Worst compound	LUFCIZ	LUFCIZ	LUFCIZ	LUFCIZ
Best compound	ONEHAS	ONEHAS	FUHWAG	ONEHAS

Pearson correlation coefficients for conformational energies

	PBE	PBE0	M06	ωB97X-V
ADULES	0.95	0.93	0.90	0.92
AJOMIX	0.81	0.89	0.81	0.71
AQINUK	0.99	0.99	0.98	0.99
AVIXIO	0.99	0.99	0.98	0.99
FIYMEI	0.83	0.83	0.74	0.54
FUDNIB	0.84	0.88	0.89	0.65
FUHWAG	0.99	0.99	0.99	0.99
LIBLEN	0.98	0.97	0.94	0.97
LUFCIZ	0.42	0.68	0.65	0.36
ONEHAS	0.99	1.00	0.98	0.99
OQOQOB	0.98	0.99	0.98	0.98
QUHVAS	0.97	0.98	0.96	0.96
ROBHUN	0.99	0.99	0.99	0.99
UZEYAA	0.93	0.96	0.91	0.93
WUDYOL	0.99	0.99	0.98	0.97
YIKLUC	0.98	0.99	0.99	0.99

Table S2. Table forming the basis of Figure 3.

Mean correlation coefficients for PBEh-3c.

	average	min	max
ADULES	0.86	0.80	0.90
AJOMIX	0.35	0.06	0.55
AQINUK	0.99	0.98	0.99
AVIXIO	0.99	0.98	0.99
FIYMEI	0.85	0.69	0.95
FUDNIB	0.92	0.78	0.98
FUHWAG	0.99	0.98	0.99
LIBLEN	0.93	0.84	0.97
LUFCIZ	0.72	0.38	0.96
ONEHAS	0.99	0.98	1.00
OQOQOB	0.91	0.87	0.95
QUHVAS	0.96	0.94	0.98
ROBHUN	0.98	0.97	0.99
UZEYAA	0.93	0.89	0.95

WUDYOL	0.98	0.96	0.99
YIKLUC	0.98	0.97	0.99

Mean correlation coefficients for B97-3c.

	average	**min**	**max**
ADULES	0.96	0.94	1.00
AJOMIX	0.88	0.68	0.98
AQINUK	0.99	0.98	1.00
AVIXIO	0.99	0.98	1.00
FIYMEI	0.88	0.61	0.99
FUDNIB	0.90	0.64	0.99
FUHWAG	0.99	0.99	1.00
LIBLEN	0.95	0.89	0.98
LUFCIZ	0.72	0.28	0.95
ONEHAS	1.00	0.99	1.00
OQOQOB	0.99	0.99	1.00
QUHVAS	0.98	0.97	1.00
ROBHUN	0.99	0.98	1.00
UZEYAA	0.95	0.90	1.00
WUDYOL	0.99	0.98	1.00
YIKLUC	0.99	0.98	1.00

Correlation coefficients for PBEh-3c.

	PBE	**PBE0**	**M06**	**ωB97X-V**
ADULES	0.85	0.80	0.87	0.90
AJOMIX	0.06	0.35	0.55	0.46
AQINUK	0.99	0.99	0.98	0.99
AVIXIO	0.99	0.99	0.99	0.98
FIYMEI	0.92	0.95	0.85	0.69
FUDNIB	0.95	0.98	0.98	0.78
FUHWAG	0.99	0.99	0.98	0.98
LIBLEN	0.94	0.97	0.84	0.97
LUFCIZ	0.38	0.96	0.68	0.86
ONEHAS	1.00	1.00	0.98	1.00
OQOQOB	0.87	0.92	0.91	0.95
QUHVAS	0.94	0.95	0.95	0.98
ROBHUN	0.97	0.98	0.97	0.99
UZEYAA	0.92	0.94	0.89	0.95
WUDYOL	0.98	0.99	0.99	0.96
YIKLUC	0.97	0.98	0.99	0.98

Correlation coefficients for B97-3c.

	PBE	**PBE0**	**M06**	**ωB97X-V**
ADULES	1.00	0.94	0.94	0.96
AJOMIX	0.97	0.98	0.90	0.68
AQINUK	1.00	1.00	0.98	0.99
AVIXIO	1.00	0.99	0.98	0.99
FIYMEI	0.99	0.99	0.93	0.61

FUDNIB	0.99	0.99	0.98	0.64
FUHWAG	0.99	1.00	0.99	1.00
LIBLEN	0.98	0.97	0.89	0.97
LUFCIZ	0.94	0.71	0.95	0.28
ONEHAS	1.00	1.00	0.99	1.00
OQOQOB	0.99	1.00	0.99	0.99
QUHVAS	1.00	1.00	0.97	0.97
ROBHUN	1.00	0.99	0.98	0.98
UZEYAA	1.00	0.99	0.90	0.93
WUDYOL	0.99	1.00	0.99	0.98
YIKLUC	1.00	1.00	0.98	0.98

Table S3. Table forming the basis of Figure 4.

Mean correlation coefficients for PM6.

	average	**min**	**max**
ADULES	0.94	0.89	0.98
AJOMIX	0.24	0.00	0.47
AQINUK	-0.14	-0.19	-0.12
AVIXIO	0.61	0.56	0.65
FIYMEI	-0.42	-0.65	-0.05
FUDNIB	0.46	0.38	0.54
FUHWAG	0.60	0.53	0.65
LIBLEN	0.63	0.58	0.68
LUFCIZ	0.16	-0.59	0.79
ONEHAS	0.69	0.67	0.75
OQOQOB	0.02	-0.02	0.07
QUHVAS	0.93	0.91	0.97
ROBHUN	0.82	0.78	0.85
UZEYAA	0.84	0.78	0.90
WUDYOL	0.94	0.92	0.96
YIKLUC	0.72	0.65	0.78

Mean correlation coefficients for PM7.

	average	**min**	**max**
ADULES	0.94	0.89	0.97
AJOMIX	0.51	0.28	0.73
AQINUK	-0.11	-0.17	-0.08
AVIXIO	0.95	0.94	0.95
FIYMEI	-0.03	-0.26	0.16
FUDNIB	0.34	-0.07	0.57
FUHWAG	0.97	0.96	0.97
LIBLEN	0.09	0.05	0.20
LUFCIZ	0.33	-0.36	0.86
ONEHAS	0.95	0.93	0.97
OQOQOB	0.83	0.81	0.84
QUHVAS	0.81	0.75	0.85
ROBHUN	0.64	0.61	0.65

UZEYAA	0.71	0.69	0.75
WUDYOL	0.05	0.03	0.10
YIKLUC	0.82	0.79	0.87

Correlation coefficients for PM6.

	PBE	PBE0	M06	ωB97X-V
ADULES	0.98	0.92	0.89	0.97
AJOMIX	0.47	0.24	0.00	0.25
AQINUK	-0.12	-0.12	-0.12	-0.19
AVIXIO	0.63	0.61	0.65	0.56
FIYMEI	-0.60	-0.65	-0.38	-0.05
FUDNIB	0.38	0.50	0.54	0.43
FUHWAG	0.65	0.65	0.53	0.57
LIBLEN	0.68	0.64	0.58	0.63
LUFCIZ	0.79	-0.09	0.52	-0.59
ONEHAS	0.68	0.69	0.75	0.67
OQOQOB	-0.02	0.00	0.07	0.05
QUHVAS	0.93	0.92	0.91	0.97
ROBHUN	0.83	0.85	0.78	0.84
UZEYAA	0.84	0.85	0.78	0.90
WUDYOL	0.96	0.94	0.95	0.92
YIKLUC	0.65	0.72	0.74	0.78

Correlation coefficients for PM7.

	PBE	PBE0	M06	ωB97X-V
ADULES	0.93	0.97	0.89	0.96
AJOMIX	0.73	0.60	0.43	0.28
AQINUK	-0.11	-0.10	-0.08	-0.17
AVIXIO	0.95	0.95	0.94	0.94
FIYMEI	0.05	-0.06	0.16	-0.26
FUDNIB	0.57	0.46	0.39	-0.07
FUHWAG	0.97	0.97	0.96	0.97
LIBLEN	0.07	0.06	0.20	0.05
LUFCIZ	0.86	0.12	0.68	-0.36
ONEHAS	0.93	0.94	0.97	0.94
OQOQOB	0.84	0.83	0.81	0.83
QUHVAS	0.81	0.85	0.82	0.75
ROBHUN	0.65	0.63	0.61	0.65
UZEYAA	0.69	0.70	0.75	0.69
WUDYOL	0.10	0.05	0.04	0.03
YIKLUC	0.79	0.83	0.81	0.87

Table S4. Table forming the basis of Figure 5.

Mean correlation coefficients for GFN1-xTB.

	average	min	max
ADULES	0.95	0.93	0.97

AJOMIX	0.57	0.20	0.82
AQINUK	0.25	0.24	0.26
AVIXIO	0.97	0.95	0.98
FIYMEI	0.35	-0.05	0.55
FUDNIB	0.78	0.40	0.92
FUHWAG	0.96	0.95	0.98
LIBLEN	-0.01	-0.06	0.05
LUFCIZ	0.62	0.19	0.88
ONEHAS	0.98	0.98	0.99
OQOQOB	0.91	0.90	0.92
QUHVAS	0.95	0.94	0.96
ROBHUN	0.78	0.73	0.82
UZEYAA	0.76	0.66	0.80
WUDYOL	0.93	0.90	0.95
YIKLUC	-	-	-

Mean correlation coefficients for GFN2-xTB.

	average	**min**	**max**
ADULES	0.97	0.93	0.98
AJOMIX	0.77	0.42	0.91
AQINUK	0.31	0.27	0.33
AVIXIO	0.92	0.89	0.93
FIYMEI	0.81	0.46	0.93
FUDNIB	0.76	0.45	0.89
FUHWAG	0.97	0.95	0.98
LIBLEN	0.62	0.56	0.66
LUFCIZ	0.25	-0.40	0.72
ONEHAS	0.97	0.96	0.97
OQOQOB	0.76	0.74	0.79
QUHVAS	0.96	0.95	0.97
ROBHUN	0.77	0.73	0.80
UZEYAA	0.87	0.82	0.91
WUDYOL	0.97	0.95	0.99
YIKLUC	0.95	0.94	0.95

Mean correlation coefficients for GFN-FF.

	average	**min**	**max**
ADULES	0.93	0.90	0.97
AJOMIX	-0.10	-0.35	0.11
AQINUK	0.49	0.48	0.50
AVIXIO	0.90	0.88	0.91
FIYMEI	0.40	0.02	0.58
FUDNIB	0.13	0.04	0.24
FUHWAG	0.98	0.98	0.98
LIBLEN	0.30	0.15	0.36
LUFCIZ	0.06	-0.60	0.75
ONEHAS	0.98	0.97	0.99
OQOQOB	0.96	0.94	0.98
QUHVAS	0.82	0.78	0.84

ROBHUN	0.58	0.55	0.61
UZEYAA	0.83	0.78	0.86
WUDYOL	0.93	0.90	0.95
YIKLUC	0.76	0.69	0.81

Correlation coefficients for GFN1-xTB.

	PBE	**PBE0**	**M06**	**ωB97X-V**
ADULES	0.97	0.96	0.93	0.96
AJOMIX	0.82	0.69	0.56	0.20
AQINUK	0.26	0.26	0.25	0.24
AVIXIO	0.98	0.98	0.95	0.97
FIYMEI	0.52	0.55	0.38	-0.05
FUDNIB	0.92	0.91	0.88	0.40
FUHWAG	0.95	0.96	0.97	0.98
LIBLEN	0.05	-0.06	0.03	-0.06
LUFCIZ	0.19	0.88	0.60	0.80
ONEHAS	0.98	0.99	0.98	0.99
OQOQOB	0.92	0.92	0.90	0.91
QUHVAS	0.95	0.94	0.95	0.96
ROBHUN	0.73	0.79	0.77	0.82
UZEYAA	0.80	0.80	0.66	0.78
WUDYOL	0.95	0.94	0.94	0.90
YIKLUC	-	-	-	-

Correlation coefficients for GFN2-xTB.

	PBE	**PBE0**	**M06**	**ωB97X-V**
ADULES	0.98	0.97	0.93	0.97
AJOMIX	0.91	0.89	0.84	0.42
AQINUK	0.33	0.33	0.32	0.27
AVIXIO	0.92	0.93	0.89	0.92
FIYMEI	0.93	0.93	0.91	0.46
FUDNIB	0.89	0.89	0.84	0.45
FUHWAG	0.95	0.95	0.98	0.98
LIBLEN	0.66	0.63	0.56	0.61
LUFCIZ	-0.40	0.58	0.10	0.72
ONEHAS	0.97	0.97	0.96	0.97
OQOQOB	0.79	0.75	0.75	0.74
QUHVAS	0.96	0.95	0.95	0.97
ROBHUN	0.73	0.76	0.78	0.80
UZEYAA	0.87	0.91	0.82	0.90
WUDYOL	0.99	0.98	0.98	0.95
YIKLUC	0.94	0.95	0.95	0.95

Correlation coefficients for GFN-FF.

	PBE	**PBE0**	**M06**	**ωB97X-V**
ADULES	0.97	0.90	0.91	0.96
AJOMIX	-0.35	-0.12	0.11	-0.06
AQINUK	0.50	0.49	0.48	0.50

AVIXIO	0.91	0.90	0.88	0.91
FIYMEI	0.52	0.58	0.47	0.02
FUDNIB	0.04	0.14	0.10	0.24
FUHWAG	0.98	0.98	0.98	0.98
LIBLEN	0.36	0.36	0.15	0.33
LUFCIZ	0.75	-0.25	0.34	-0.60
ONEHAS	0.98	0.98	0.97	0.99
OQOQOB	0.98	0.97	0.96	0.94
QUHVAS	0.82	0.78	0.84	0.83
ROBHUN	0.55	0.57	0.59	0.61
UZEYAA	0.86	0.85	0.78	0.83
WUDYOL	0.95	0.93	0.94	0.90
YIKLUC	0.69	0.75	0.78	0.81

Table S5. Table forming the basis of Figure 6.

	Q3	**Q1**	**max**	**min**	**median**
PBE-D3(BJ)	0.99	0.91	0.99	0.42	0.98
PBE0-D3(BJ)	0.99	0.92	1.00	0.68	0.98
M06	0.98	0.90	0.99	0.65	0.97
ωB97X-V	0.99	0.87	0.99	0.36	0.97
PBEh-3c	0.98	0.90	0.99	0.35	0.94
B97-3c	0.99	0.94	1.00	0.72	0.99
PM6	0.83	0.22	0.94	-0.42	0.62
PM7	0.86	0.27	0.97	-0.11	0.67
GFN1-xTB	0.95	0.59	0.98	-0.01	0.78
GFN2-xTB	0.96	0.76	0.97	0.25	0.84
GFN-FF	0.93	0.37	0.98	-0.10	0.79

Table S6. Table forming the basis of Figure 7.

	τ,s
PBE-D3(BJ)	191.554
PBE0-D3(BJ)	2833.729
M06	2985.011
ωB97X-V	5083.924
B97-3c	89.404
PBEh-3c	732.035
GFN1	0.102
GFN2	0.045
GFN-FF	0.002
PM6	0.06
PM7	0.06

Computer architecture: Intel(R) Core(TM) i5-10600K CPU @ 4.10GHz, 12 Gb RAM. Single core was utilized.

Table S7. Table forming the basis of Figure 8.

Pearson correlation coefficients for the compounds of 16OSTM10 database.

	ρ(PBE/λ2,PBE-D3/λ2)
ADULES	0.98
AJOMIX	0.83
AQINUK	0.97
AVIXIO	-0.03
FIYMEI	0.43
FUDNIB	0.57
FUHWAG	0.82
LIBLEN	0.96
LUFCIZ	0.90
ONEHAS	0.99
OQOQOB	0.36
QUHVAS	0.97
ROBHUN	0.97
UZEYAA	0.96
WUDYOL	0.98
YIKLUC	1.00

Absolute energies of the conformations.

	E(PBE/λ2), Hartree	*E*(PBE-D3/λ2), Hartree
AQINUK_13	-14773.18958987	-14773.39572320
AQINUK_15	-14773.18909685	-14773.39552260
AQINUK_17	-14773.19006450	-14773.39754890
AQINUK_20	-14773.18209972	-14773.39202320
AQINUK_22	-14773.18803601	-14773.39488890
AQINUK_29	-14773.18532039	-14773.39373860
AQINUK_32	-14773.19374792	-14773.39866630
AQINUK_6	-14773.19137329	-14773.39682680
AQINUK_7	-14773.18870787	-14773.39502500
AQINUK_9	-14773.19005499	-14773.39643980
AVIXIO_10	-9169.07080765	-9169.39987730
AVIXIO_13	-9169.06718954	-9169.41365544
AVIXIO_14	-9169.05921435	-9169.39063622
AVIXIO_18	-9169.06941891	-9169.38825686
AVIXIO_1	-9169.06659658	-9169.40484071
AVIXIO_20	-9169.07301828	-9169.39140229
AVIXIO_21	-9169.05871940	-9169.39329549
AVIXIO_29	-9169.06583520	-9169.40183112
AVIXIO_6	-9169.06861715	-9169.37467736
AVIXIO_7	-9169.06432069	-9169.39715459
FUHWAG_14	-5610.75066424	-5611.06911273
FUHWAG_15	-5610.76285951	-5611.08308297
FUHWAG_27	-5610.76084649	-5611.08836039
FUHWAG_31	-5610.75217648	-5611.05050731

FUHWAG_32	-5610.72998715	-5611.05610486
FUHWAG_33	-5610.75733521	-5611.07626111
FUHWAG_34	-5610.72692895	-5611.03402162
FUHWAG_3	-5610.75776431	-5611.07501040
FUHWAG_6	-5610.75241487	-5611.05682053
FUHWAG_8	-5610.76168456	-5611.07307748
OQOQOB_10	-6284.93613798	-6285.28693455
OQOQOB_13	-6284.93992218	-6285.30791036
OQOQOB_17	-6284.93206104	-6285.26427936
OQOQOB_1	-6284.93906166	-6285.28292884
OQOQOB_22	-6284.92968058	-6285.27806728
OQOQOB_26	-6284.93884803	-6285.26721225
OQOQOB_30	-6284.93421247	-6285.28266902
OQOQOB_3	-6284.93443704	-6285.28502328
OQOQOB_6	-6284.95258933	-6285.27274288
OQOQOB_8	-6284.95766487	-6285.30261991
WUDYOL_0	-3365.92567093	-3366.04385828
WUDYOL_16	-3365.92633909	-3366.04424275
WUDYOL_19	-3365.92465111	-3366.04352511
WUDYOL_20	-3365.92458616	-3366.04153828
WUDYOL_21	-3365.92417380	-3366.04217666
WUDYOL_32	-3365.91831691	-3366.03715427
WUDYOL_34	-3365.91526920	-3366.03412316
WUDYOL_3	-3365.92274571	-3366.03971021
WUDYOL_7	-3365.91766403	-3366.03718520
WUDYOL_8	-3365.91824895	-3366.03746748
YIKLUC_15	-2947.60179050	-2947.76280711
YIKLUC_18	-2947.60146966	-2947.76289800
YIKLUC_19	-2947.60191833	-2947.76320955
YIKLUC_27	-2947.60490643	-2947.76733277
YIKLUC_29	-2947.59464934	-2947.75565699
YIKLUC_30	-2947.60490877	-2947.76644897
YIKLUC_32	-2947.59925495	-2947.75987496
YIKLUC_33	-2947.60087199	-2947.76217573
YIKLUC_34	-2947.59694240	-2947.75763625
YIKLUC_9	-2947.60617699	-2947.76834241
LIBLEN_16	-2728.89037254	-2729.03958725
LIBLEN_18	-2728.89052564	-2729.03964391
LIBLEN_1	-2728.89612672	-2729.04336249
LIBLEN_23	-2728.89052627	-2729.04016380
LIBLEN_24	-2728.88899990	-2729.03526877
LIBLEN_25	-2728.88368277	-2729.03230438
LIBLEN_26	-2728.89053615	-2729.03910705
LIBLEN_31	-2728.88409753	-2729.03322960
LIBLEN_33	-2728.89502980	-2729.04172213
LIBLEN_3	-2728.89564956	-2729.04289863
ONEHAS_12	-3244.41006970	-3244.63082024
ONEHAS_14	-3244.41199479	-3244.63092203
ONEHAS_17	-3244.40329840	-3244.62429939
ONEHAS_22	-3244.40357900	-3244.62417748

ONEHAS_23	-3244.39875918	-3244.61790303
ONEHAS_27	-3244.38353377	-3244.60588665
ONEHAS_30	-3244.38208145	-3244.60409414
ONEHAS_31	-3244.38635711	-3244.61205569
ONEHAS_33	-3244.40131212	-3244.62495600
ONEHAS_34	-3244.38245547	-3244.60442146
UZEYAA_14	-3891.83024091	-3892.07160777
UZEYAA_19	-3891.83008407	-3892.07012319
UZEYAA_20	-3891.84112263	-3892.07972428
UZEYAA_22	-3891.83113304	-3892.07100437
UZEYAA_23	-3891.84015508	-3892.07572665
UZEYAA_30	-3891.83533515	-3892.07400234
UZEYAA_31	-3891.83922215	-3892.07743790
UZEYAA_33	-3891.83133269	-3892.07168807
UZEYAA_3	-3891.83425407	-3892.07288898
UZEYAA_7	-3891.84129394	-3892.07888925
ADULES_14	-3092.51201732	-3092.69304940
ADULES_16	-3092.52774329	-3092.70314664
ADULES_20	-3092.52530924	-3092.70151279
ADULES_23	-3092.51665397	-3092.69640612
ADULES_25	-3092.51669377	-3092.69508230
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ADULES_2	-3092.52173770	-3092.69886801
ADULES_31	-3092.51448295	-3092.69242929
ADULES_6	-3092.51951173	-3092.69592108
ADULES_9	-3092.51132739	-3092.69093187
AJOMIX_11	-4476.60604917	-4476.81202450
AJOMIX_14	-4476.60348911	-4476.81010973
AJOMIX_17	-4476.60267220	-4476.81039517
AJOMIX_18	-4476.60739914	-4476.81403947
AJOMIX_19	-4476.60713589	-4476.81409206
AJOMIX_26	-4476.60701163	-4476.81387462
AJOMIX_31	-4476.60462004	-4476.81035596
AJOMIX_4	-4476.60592395	-4476.80938065
AJOMIX_7	-4476.60351552	-4476.80952930
AJOMIX_9	-4476.60756533	-4476.81400623
FIYMEI_10	-6434.49058795	-6434.80956262
FIYMEI_12	-6434.48044361	-6434.79860198
FIYMEI_17	-6434.48150501	-6434.79525908
FIYMEI_18	-6434.47772465	-6434.79617935
FIYMEI_21	-6434.47954657	-6434.81717111
FIYMEI_28	-6434.47881272	-6434.80670693
FIYMEI_31	-6434.48669340	-6434.80573867
FIYMEI_32	-6434.47364428	-6434.79594755
FIYMEI_5	-6434.47955659	-6434.80067479
FIYMEI_6	-6434.48020046	-6434.79970603
QUHVAS_16	-3411.99095636	-3412.18980991
QUHVAS_20	-3411.98806832	-3412.18811247
QUHVAS_21	-3411.98453617	-3412.18689936
QUHVAS_24	-3411.97124149	-3412.17404124

QUHVAS_25	-3411.98184796	-3412.18497682
QUHVAS_26	-3411.97995692	-3412.17903192
QUHVAS_27	-3411.97377877	-3412.17897882
QUHVAS_28	-3411.99235346	-3412.19024210
QUHVAS_29	-3411.96954857	-3412.17393631
QUHVAS_6	-3411.98243012	-3412.18372402
FUDNIB_18	-4541.58506057	-4541.80985694
FUDNIB_21	-4541.58556205	-4541.80770346
FUDNIB_23	-4541.58607438	-4541.80607285
FUDNIB_24	-4541.58461327	-4541.80242194
FUDNIB_26	-4541.58238413	-4541.80499325
FUDNIB_27	-4541.58650860	-4541.81286286
FUDNIB_2	-4541.58745213	-4541.80775509
FUDNIB_32	-4541.58676239	-4541.81300568
FUDNIB_3	-4541.58645492	-4541.81243594
FUDNIB_5	-4541.58549864	-4541.80523584
LUFCIZ_25	-3592.17307904	-3592.42059437
LUFCIZ_27	-3592.16736935	-3592.41030929
LUFCIZ_28	-3592.16649064	-3592.41602369
LUFCIZ_29	-3592.16753941	-3592.41892177
LUFCIZ_2	-3592.18077240	-3592.43006424
LUFCIZ_30	-3592.16113583	-3592.41396696
LUFCIZ_32	-3592.16062592	-3592.41046575
LUFCIZ_6	-3592.17104859	-3592.42273467
LUFCIZ_9	-3592.17379822	-3592.42547364
ROBHUN_10	-5594.49325700	-5594.70774467
ROBHUN_12	-5594.49457945	-5594.70950435
ROBHUN_13	-5594.48992405	-5594.70308577
ROBHUN_14	-5594.49696543	-5594.71206300
ROBHUN_29	-5594.49617789	-5594.71073301
ROBHUN_2	-5594.49655413	-5594.71025193
ROBHUN_34	-5594.48978930	-5594.70282712
ROBHUN_3	-5594.49595350	-5594.70885132
ROBHUN_4	-5594.50058495	-5594.71432033
ROBHUN_8	-5594.49378397	-5594.70896207

Table S8. T1/T2 diagnostic values for 10 compounds of 16OSTM10 database

	T1	T2
LUFCIZ	0.011	0.063
ONEHAS	0.012	0.047
ROBHUN	0.012	0.058
ADULES	0.012	0.080
AQINUK	0.012	0.078
AVIXIO	0.013	0.071
FUHWAG	0.013	0.072
OQOQOB	0.013	0.073
QUHVAS	0.013	0.094
WUDYOL	0.017	0.093

FOD plots

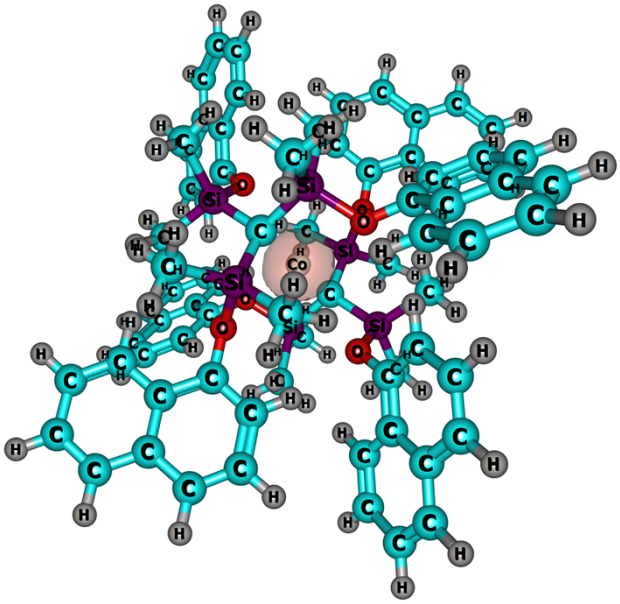

Figure S1. Qualitative FOD diagnostics for FIYMEI. The isosurface value is σ = 0.005 e/Bohr^3.

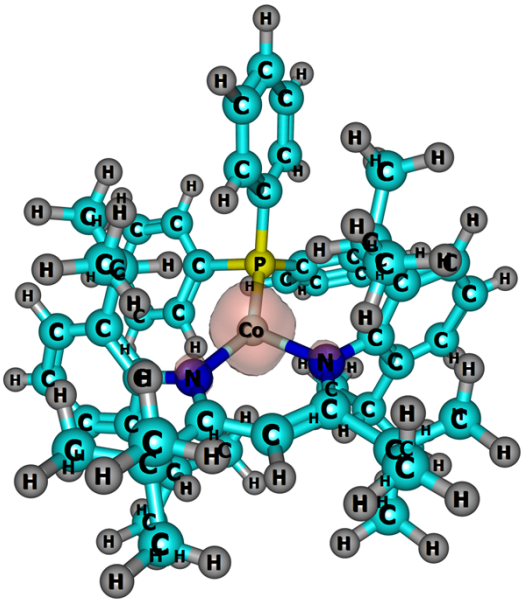

Figure S2. Qualitative FOD diagnostics for UZEYAA. The isosurface value is σ = 0.005 e/Bohr^3.

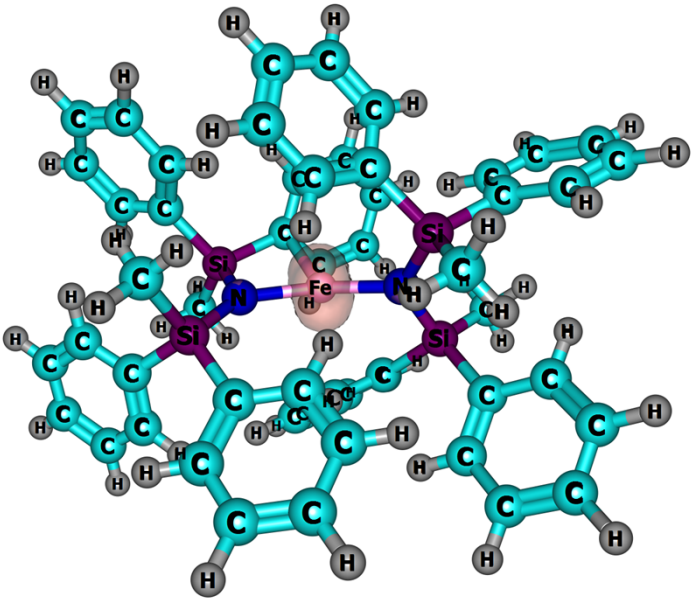

Figure S3. Qualitative FOD diagnostics for FUDNIB. The isosurface value is σ = 0.005 e/Bohr^3.

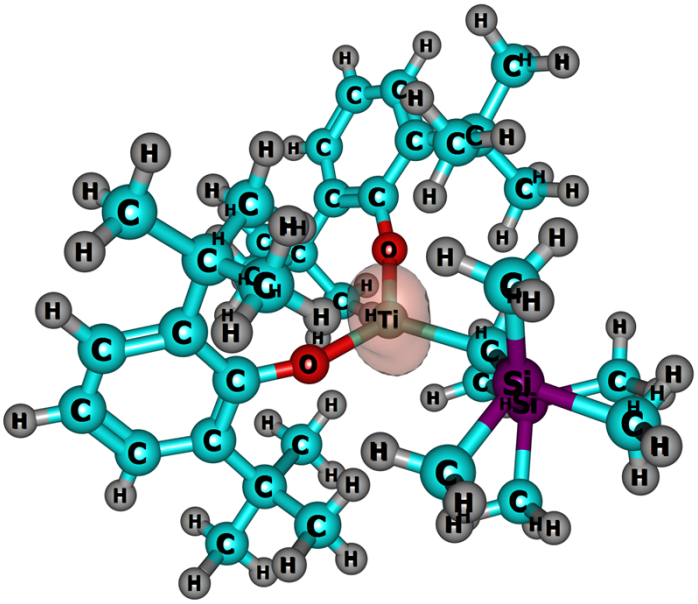

Figure S4. Qualitative FOD diagnostics for YIKLUC. The isosurface value is σ = 0.005 e/Bohr^3.

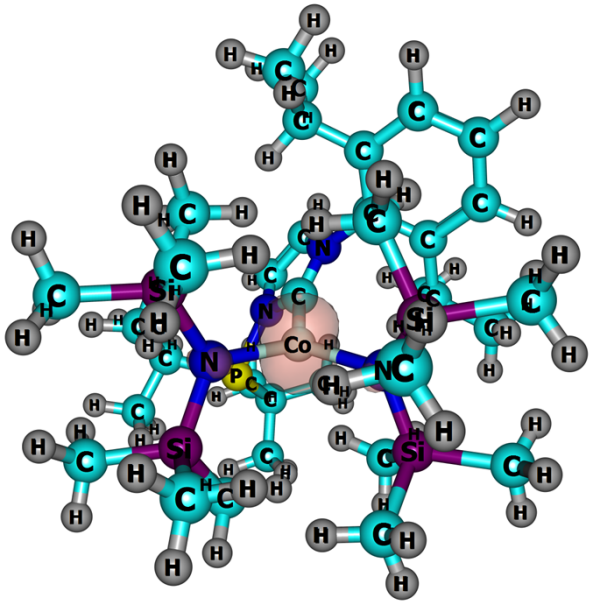

Figure S5. Qualitative FOD diagnostics for AJOMIX. The isosurface value is σ = 0.005 e/Bohr^3.

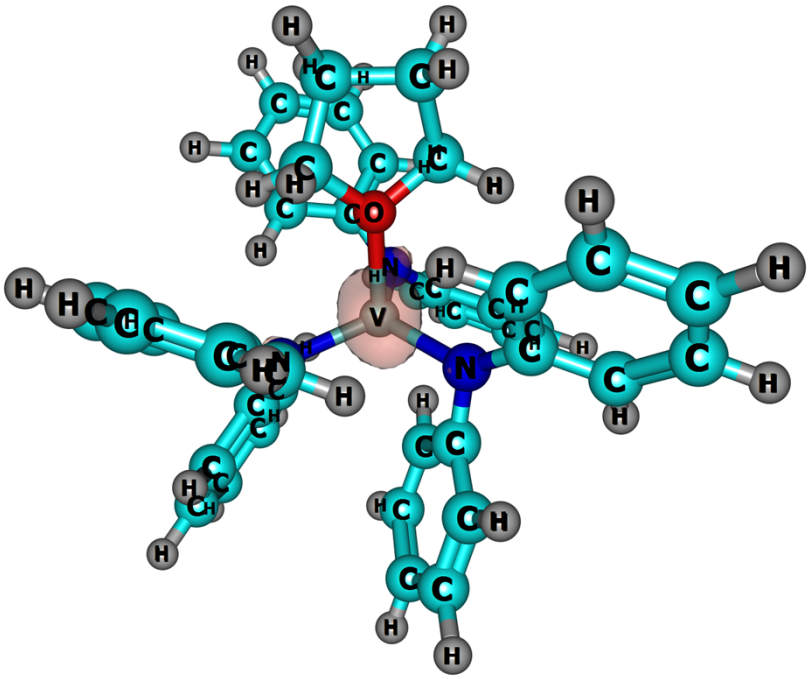

Figure S6. Qualitative FOD diagnostics for LIBLEN. The isosurface value is σ = 0.005 e/Bohr^3.

Composition of the λ1 and λ2 basis sets used in the Priroda calculations

Elements	Primitive and contracted functions
λ1	
H	(6s2p) → [2s1p]
B, C, N, O, F	(10s7p3d) → [3s2p1d]
Al, Si, P, S, Cl	(14s11p3d) → [4s3p1d]
Ti, V, Cr, Fe, Co, Cu	(19s15p11d5f) → [6s5p3d1f]
Br	(19s15p11d) → [5s4p2d]
λ2	
H	(8s4p2d) → [3s2p1d]
B, C, N, O, F	(12s8p4d2f) → [4s3p2d1f]
Al, Si, P, S, Cl	(18s13p5d2f) → [5s4p2d1f]
Ti, V, Cr, Fe, Co, Cu	(23s18p13d8f4g) → [8s7p5d3f1g]
Br	(23s18p13d2f) → [6s5p3d1f]
λ1 (relativistic)	
H	(6s2p) → [2s1p]
B, C, N, O, F	(10s7p3d) → [3s2p1d]
Al, Si, P, S, Cl	(15s11p3d) → [4s3p1d]
Ti, V, Cr, Fe, Co, Cu	(21s16p11d5f) → [6s5p3d1f]
Br	(21s17p11d) → [5s4p2d]
λ2 (relativistic)	
H	(8s4p2d) → [3s2p1d]
B, C, N, O, F	(12s8p4d2f) → [4s3p2d1f]
Al, Si, P, S, Cl	(19s13p5d2f) → [5s4p2d1f]
Ti, V, Cr, Fe, Co, Cu	(25s20p14d8f4g) → [8s7p5d3f1g]
Br	(25s21p14d2f) → [6s5p3d1f]

Tabulated absolute conformational energies and optimized Cartesian coordinates for the compounds of 16OSTM10 database.

ADULES

Conformation 14.
Multiplicity: 4
Charge: 0
E(B97-3c) = -3093.966599795127 Hartree
E(M06/def2-TZVP) = -3093.636197040315 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3092.607314558257 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3092.835883758034 Hartree
E(PBEh-3c) = -3089.871015364763 Hartree
E(PM6) = 12.97362 Kcal/mol
E(PM7) = 12.80835 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3095.693463217948 Hartree
E(GFN1-xTB) = -132.177647242737 Hartree
E(GFN2-xTB) = -130.925202510276 Hartree
E(GFN-FF) = -18.182891646888 Hartree

Coordinates:

Co	-0.524023	0.313364	-0.282308
C	-2.133803	1.496291	-0.467672
H	-1.885718	2.421581	-1.037301
H	-2.737215	0.868477	-1.165412
C	-2.960112	1.852405	0.768044
H	-3.914745	2.347536	0.460819
H	-3.283656	0.922686	1.283221
C	-2.241343	2.774228	1.759163
H	-1.892325	3.668343	1.197422
H	-1.312586	2.279700	2.111553
C	-3.047517	3.251715	2.977195
H	-2.527274	4.140281	3.395558
H	-4.046778	3.618969	2.646296
C	-3.230838	2.248123	4.129660
H	-3.564957	2.813945	5.026994
H	-2.233387	1.832789	4.398267
C	-4.221634	1.104073	3.893184
H	-5.209805	1.490946	3.566660
H	-4.383751	0.516331	4.820223
H	-3.877448	0.396101	3.113341
N	-0.193693	-1.125092	-1.564675
N	1.261664	0.452191	0.491321
C	1.172595	-3.136628	-2.400775
C	0.966794	-1.789674	-1.625786
C	2.081135	-1.382393	-0.846847
H	2.970236	-1.992633	-1.008613
C	2.257583	-0.379150	0.141297
C	3.714114	-0.322241	0.722379
C	0.118053	-3.461210	-3.476531
H	0.385397	-4.430334	-3.945119
H	0.077745	-2.701035	-4.276030
H	-0.899252	-3.561911	-3.064004
C	2.554657	-3.189671	-3.095874
H	2.632155	-4.125965	-3.684598
H	3.402319	-3.187106	-2.384218
H	2.694836	-2.339826	-3.792481
C	1.117613	-4.256407	-1.329418
H	1.255726	-5.248237	-1.808515
H	0.139735	-4.264463	-0.809129
H	1.906917	-4.126367	-0.563122
C	4.635564	0.161935	-0.424048
H	5.686728	0.218005	-0.071993
H	4.336170	1.172173	-0.769264
H	4.598871	-0.515881	-1.298575
C	4.153855	-1.733521	1.185755
H	3.460877	-2.130136	1.955512
H	5.165451	-1.677084	1.637105
H	4.201937	-2.470665	0.362276
C	3.942461	0.607754	1.929271
H	3.358359	0.301635	2.816456
H	3.701488	1.663132	1.720189
H	5.016559	0.557527	2.201671
C	-1.329529	-1.191209	-2.407251
C	-1.378847	-0.376396	-3.579841
C	-2.558004	-0.399984	-4.348459
H	-2.601337	0.218870	-5.259371
C	-3.673491	-1.160411	-3.977066
H	-4.582161	-1.152192	-4.597417
C	-3.631248	-1.903568	-2.791816
H	-4.517519	-2.477101	-2.478042
C	-2.479099	-1.926152	-1.988248
C	-0.250105	0.535799	-4.074476
H	-0.763873	1.247450	-4.756630
C	0.792684	-0.201098	-4.931942
H	0.316835	-0.807591	-5.728421
H	1.416539	-0.872134	-4.310604
H	1.474901	0.527122	-5.417566
C	0.450869	1.396366	-3.012058
H	-0.276842	1.891299	-2.339416
H	1.037861	2.198291	-3.506303
H	1.159806	0.809979	-2.395038
C	-2.488712	-2.708615	-0.679725
H	-1.467590	-2.636781	-0.249650
C	-2.807603	-4.199331	-0.885013
H	-2.117054	-4.674421	-1.609518
H	-3.840494	-4.344316	-1.263772
H	-2.727442	-4.750555	0.074456
C	-3.465796	-2.079235	0.329026
H	-3.227010	-1.013610	0.509993
H	-3.429388	-2.611091	1.302246
H	-4.509958	-2.126696	-0.043150
C	1.210134	1.359027	1.580302
C	0.843076	0.867344	2.870175
C	0.721206	1.779623	3.929786
H	0.447976	1.414599	4.930645
C	0.938092	3.152000	3.732622
H	0.834320	3.852825	4.574451
C	1.272801	3.625259	2.458670
H	1.432264	4.704286	2.307020
C	1.414087	2.751100	1.365505
C	0.530905	-0.612974	3.044842
H	1.177417	-1.170619	2.335994
C	-0.926774	-0.888373	2.636852
H	-1.135867	-1.973474	2.550979
H	-1.174833	-0.412112	1.656423
H	-1.634891	-0.446111	3.366475
C	0.815389	-1.155293	4.449636
H	0.665530	-2.253540	4.476553
H	0.135835	-0.717177	5.209427
H	1.857514	-0.943205	4.763664
C	1.794549	3.293760	-0.006493
H	1.864000	2.421809	-0.687888
C	0.711082	4.234078	-0.559190
H	-0.274651	3.732425	-0.586230
H	0.962707	4.561167	-1.588980
H	0.609586	5.143800	0.068567
C	3.166170	3.990625	0.005303
H	3.967192	3.321125	0.376908
H	3.158239	4.892654	0.652057
H	3.444819	4.318072	-1.017528

Conformation 16.
Multiplicity: 4
Charge: 0
E(B97-3c) = -3093.978690751810 Hartree
E(M06/def2-TZVP) = -3093.642591378878 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3092.617752475290 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3092.841386704271 Hartree
E(PBEh-3c) = -3089.876407988302 Hartree
E(PM6) = 2.70757 Kcal/mol
E(PM7) = 7.79350 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3095.703850570486 Hartree
E(GFN1-xTB) = -132.188639001650 Hartree
E(GFN2-xTB) = -130.938520100297 Hartree
E(GFN-FF) = -18.195611646942 Hartree

Coordinates:

Co	-0.083465	0.571433	-0.016518
C	-1.800136	1.560192	0.155315
H	-1.565215	2.246802	1.006881
H	-1.900516	2.206356	-0.746340
C	-3.073567	0.772835	0.436997
H	-3.318847	0.122016	-0.432285
H	-2.901365	0.075823	1.284263
C	-4.300600	1.647972	0.749746
H	-4.471405	2.341815	-0.102629
H	-4.066228	2.298523	1.623695
C	-5.585162	0.857775	1.033978
H	-6.446753	1.560979	1.083726
H	-5.798140	0.184001	0.172055
C	-5.548256	0.026184	2.321303
H	-5.325270	0.700382	3.179163
H	-4.699695	-0.689393	2.280543

C	-6.843769	-0.740114	2.588916
H	-7.712748	-0.054270	2.678191
H	-6.787415	-1.331118	3.526013
H	-7.069823	-1.447493	1.763092
N	1.357685	0.848207	-1.248164
N	0.575051	-1.022831	0.839738
C	3.610446	0.257804	-2.346332
C	2.453494	0.076663	-1.310169
C	2.614237	-1.024329	-0.430809
H	3.555048	-1.564362	-0.563563
C	1.771055	-1.572780	0.568709
C	2.383034	-2.806448	1.318911
C	3.613275	-0.985225	-3.269076
H	4.432803	-0.904604	-4.013155
H	2.656427	-1.067194	-3.823012
H	3.755649	-1.925975	-2.703200
C	3.519960	1.503005	-3.248019
H	4.383408	1.487715	-3.943989
H	3.570489	2.446513	-2.675606
H	2.600690	1.532924	-3.858428
C	4.960290	0.353733	-1.594062
H	5.782290	0.515453	-2.321194
H	5.200268	-0.560524	-1.018598
H	4.958957	1.208070	-0.887031
C	1.523232	-3.403488	2.449873
H	2.118385	-4.188463	2.959526
H	0.595477	-3.875897	2.082546
H	1.236939	-2.655591	3.210739
C	3.721361	-2.358298	1.961873
H	4.456497	-2.008253	1.212712
H	4.175168	-3.209252	2.510293
H	3.562539	-1.533511	2.685006
C	2.671962	-3.940717	0.306104
H	3.378914	-3.629515	-0.486964
H	1.741939	-4.288671	-0.186121
H	3.117942	-4.808720	0.833930
C	1.008047	2.032142	-1.944453
C	1.457341	3.294876	-1.449282
C	0.988059	4.461602	-2.072976
H	1.325697	5.441842	-1.705143
C	0.097054	4.402821	-3.154538
H	-0.257814	5.330472	-3.628232
C	-0.342032	3.159442	-3.624296
H	-1.045102	3.116625	-4.470700
C	0.092827	1.959245	-3.034644
C	2.389459	3.368613	-0.244423
H	2.951073	2.412240	-0.203881
C	1.574363	3.458089	1.058560
H	0.886357	2.590797	1.141345
H	0.958575	4.380611	1.082205
H	2.237318	3.453778	1.948411
C	3.418885	4.502770	-0.334438
H	3.990641	4.462207	-1.283785
H	4.140791	4.434517	0.504562
H	2.942661	5.502729	-0.270255
C	-0.409651	0.622162	-3.567767
H	0.019948	-0.168353	-2.918707
C	0.072910	0.365196	-5.005814
H	1.177197	0.414917	-5.084634
H	-0.344643	1.113496	-5.711245
H	-0.248540	-0.638189	-5.353844
C	-1.940368	0.513341	-3.473358
H	-2.282560	0.666647	-2.432326
H	-2.283387	-0.487762	-3.805356
H	-2.441364	1.268930	-4.113228
C	-0.489425	-1.497362	1.642317
C	-0.820309	-0.792560	2.839274
C	-1.906900	-1.249118	3.605272
H	-2.166110	-0.726852	4.537578
C	-2.677464	-2.343796	3.193626
H	-3.521636	-2.688248	3.809562
C	-2.390699	-2.978517	1.976209
H	-3.026140	-3.810907	1.640419
C	-1.311709	-2.569312	1.176766
C	-0.026956	0.440280	3.254565
H	0.342634	0.886083	2.301223
C	1.212940	0.095176	4.094199
H	1.776988	1.014827	4.353668
H	1.901132	-0.577010	3.547885
H	0.924054	-0.407342	5.041054
C	-0.883151	1.505496	3.949477
H	-0.305534	2.446152	4.056233
H	-1.189569	1.195070	4.970099
H	-1.802226	1.731472	3.372551
C	-1.050297	-3.198602	-0.186192
H	0.042976	-3.155201	-0.363086
C	-1.469141	-4.669440	-0.288178
H	-1.020948	-5.281244	0.521220
H	-1.140766	-5.093230	-1.258822
H	-2.570039	-4.794131	-0.237868
C	-1.704594	-2.348300	-1.288992
H	-1.362398	-1.294019	-1.222027
H	-2.809163	-2.348889	-1.187060
H	-1.445828	-2.732425	-2.297303

Conformation 2.
Multiplicity: 4
Charge: 0
E(B97-3c) = -3093.973738702698 Hartree
E(M06/def2-TZVP) = -3093.639519811665 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3092.613358754087 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3092.837677445571 Hartree
E(PBEh-3c) = -3089.872596617491 Hartree
E(PM6) = 6.30908 Kcal/mol
E(PM7) = 12.43891 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3095.698706379848 Hartree
E(GFN1-xTB) = -132.180979669625 Hartree
E(GFN2-xTB) = -130.930810468457 Hartree
E(GFN-FF) = -18.191079778321 Hartree

Coordinates:

Co	0.452602	0.297322	0.045668
C	0.782289	2.247110	-0.224105
H	0.724814	2.728845	0.777499
H	1.863152	2.279272	-0.510358
C	-0.082912	2.963848	-1.250804
H	-0.042824	2.431923	-2.226364
H	-1.145058	2.909470	-0.942683
C	0.309133	4.433009	-1.501086
H	1.387384	4.451346	-1.774358
H	0.237601	5.007606	-0.549015
C	-0.498881	5.142330	-2.603896
H	0.127732	5.948315	-3.043449
H	-0.682372	4.420485	-3.432772
C	-1.833451	5.778262	-2.181363
H	-2.245591	6.324088	-3.058630
H	-1.631268	6.560404	-1.415118
C	-2.904369	4.820538	-1.650602
H	-2.621879	4.385617	-0.670829
H	-3.071975	3.973202	-2.348104
H	-3.873212	5.342192	-1.509668
N	-0.456994	-1.061210	-0.973291
N	0.880642	-0.752269	1.596932
C	-1.235780	-3.444918	-1.467223
C	-0.555957	-2.350262	-0.576229
C	-0.027224	-2.769490	0.666297
H	-0.171449	-3.826557	0.884218
C	0.622464	-2.059703	1.714227
C	0.915279	-2.914124	2.991109
C	-1.079897	-4.863869	-0.878482
H	-1.535707	-5.590480	-1.580510
H	-1.599560	-4.980635	0.093155
H	-0.017443	-5.148995	-0.747067
C	-2.751007	-3.191640	-1.625822
H	-3.202161	-4.028218	-2.198259
H	-2.963982	-2.259997	-2.179522
H	-3.257735	-3.144031	-0.641483
C	-0.585864	-3.469603	-2.865855
H	-1.006126	-4.310146	-3.455033
H	0.510811	-3.614299	-2.799745
H	-0.784396	-2.540459	-3.427503
C	1.705780	-2.207367	4.108292
H	1.784434	-2.901953	4.969433
H	1.214580	-1.286807	4.466230
H	2.733714	-1.939746	3.804119
C	1.719715	-4.178557	2.605499
H	1.179679	-4.837703	1.899696
H	1.935758	-4.772427	3.517087
H	2.689539	-3.907100	2.141133
C	-0.453283	-3.333537	3.584496
H	-1.051082	-3.930149	2.868983
H	-1.051643	-2.442877	3.862637
H	-0.299636	-3.943775	4.498491
C	-1.063842	-0.396082	-2.073084
C	-0.301747	-0.117436	-3.250338
C	-0.888583	0.666519	-4.260271
H	-0.309454	0.888795	-5.169619
C	-2.183757	1.180270	-4.128269
H	-2.620690	1.794519	-4.929896
C	-2.915991	0.918474	-2.962645
H	-3.927235	1.337921	-2.854850
C	-2.382100	0.142035	-1.920715
C	1.140864	-0.590430	-3.408263
H	1.332516	-1.328976	-2.603041
C	2.123391	0.576338	-3.203682
H	1.985840	1.040274	-2.209797
H	1.972676	1.364324	-3.970382
H	3.172656	0.223224	-3.274828
C	1.406139	-1.270303	-4.761832
H	0.697869	-2.097172	-4.961259
H	2.434450	-1.685183	-4.788210
H	1.325527	-0.548850	-5.600873

C	-3.165844	-0.054508	-0.625085
H	-2.768585	-0.966388	-0.138671
C	-4.671483	-0.256516	-0.841239
H	-4.881762	-1.066338	-1.567943
H	-5.162303	0.666837	-1.211955
H	-5.163389	-0.519273	0.117325
C	-2.904939	1.108423	0.345750
H	-1.814014	1.237480	0.510549
H	-3.383295	0.918353	1.328452
H	-3.303575	2.062833	-0.054707
C	1.642186	0.126786	2.405581
C	0.977053	1.099327	3.209227
C	1.760020	2.042930	3.898224
H	1.261104	2.793397	4.530507
C	3.155373	2.046411	3.796143
H	3.748508	2.795961	4.341257
C	3.797036	1.090548	2.994258
H	4.893971	1.100393	2.920563
C	3.067971	0.122874	2.286407
C	-0.540148	1.107297	3.368154
H	-0.949398	0.407160	2.610788
C	-1.154027	2.491377	3.102883
H	-2.260136	2.440447	3.159377
H	-0.881542	2.872140	2.100059
H	-0.820165	3.237572	3.853065
C	-0.962008	0.596215	4.758384
H	-2.067737	0.565699	4.845955
H	-0.577829	1.260995	5.559944
H	-0.578454	-0.422996	4.959126
C	3.763208	-0.900684	1.393627
H	3.180694	-1.843224	1.466035
C	3.709302	-0.470570	-0.082023
H	2.655321	-0.336379	-0.410027
H	4.170367	-1.235768	-0.739737
H	4.237115	0.492428	-0.238659
C	5.200007	-1.221627	1.821362
H	5.257244	-1.510213	2.890442
H	5.880390	-0.359137	1.665762
H	5.598848	-2.060804	1.216723

Conformation 20.
Multiplicity: 4
Charge: 0
E(B97-3c) = -3093.976593267044 Hartree
E(M06/def2-TZVP) = -3093.641615779439 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3092.615921271834 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3092.839263194862 Hartree
E(PBEh-3c) = -3089.875640250264 Hartree
E(PM6) = 4.82982 Kcal/mol
E(PM7) = 9.45028 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3095.701208591396 Hartree
E(GFN1-xTB) = -132.186815486466 Hartree
E(GFN2-xTB) = -130.935427281578 Hartree
E(GFN-FF) = -18.195490242084 Hartree

Coordinates:

Co	0.240518	0.095806	-0.354780
C	1.647642	-0.838363	-1.396767
H	1.316596	-1.898850	-1.344256
H	1.443900	-0.496887	-2.442000
C	3.124062	-0.686425	-1.058468
H	3.410733	0.388065	-1.079016
H	3.300141	-1.013919	-0.009458
C	4.095247	-1.476103	-1.963819
H	5.131309	-1.242336	-1.634972
H	4.019930	-1.098734	-3.009165
C	3.891193	-3.004023	-1.954568
H	4.871999	-3.512957	-2.084651
H	3.533003	-3.314349	-0.945668
C	2.929024	-3.549652	-3.019399
H	3.347114	-3.329238	-4.027169
H	1.964807	-3.002135	-2.970571
C	2.665621	-5.048939	-2.881545
H	3.606312	-5.636920	-2.938667
H	1.986841	-5.422741	-3.675017
H	2.191037	-5.280123	-1.904393
N	0.142877	1.768822	0.573120
N	-1.440368	-0.634213	0.205192
C	-1.065339	3.580789	1.951799
C	-0.924642	2.175282	1.278199
C	-2.061791	1.338879	1.418706
H	-2.867818	1.777790	2.012422
C	-2.333654	0.025572	0.957987
C	-3.693498	-0.569641	1.444153
C	0.158414	4.508136	1.831316
H	-0.105338	5.489697	2.275112
H	0.461873	4.684970	0.784271
H	1.042059	4.125448	2.371277
C	-2.255387	4.306483	1.274201
H	-2.386048	5.314505	1.719392
H	-3.208427	3.756386	1.392600
H	-2.074804	4.432972	0.187823
C	-1.362204	3.408797	3.460578
H	-1.464575	4.405208	3.937488
H	-0.536582	2.873505	3.971451
H	-2.297602	2.848437	3.651185
C	-4.845190	0.386093	1.050354
H	-5.814109	-0.041316	1.380869
H	-4.890352	0.518171	-0.049788
H	-4.751515	1.389483	1.507672
C	-3.623005	-0.700232	2.985265
H	-2.789091	-1.366259	3.285031
H	-4.566504	-1.136307	3.374265
H	-3.467751	0.277314	3.481403
C	-4.055851	-1.953916	0.875545
H	-3.312275	-2.730645	1.124120
H	-4.171412	-1.943054	-0.223023
H	-5.026536	-2.265986	1.311785
C	1.431651	2.332506	0.415011
C	2.395195	2.213032	1.463960
C	3.693589	2.693438	1.236020
H	4.444919	2.615081	2.035582
C	4.053856	3.267808	0.007915
H	5.076832	3.642118	-0.147307
C	3.111803	3.346027	-1.024801
H	3.405201	3.777467	-1.993687
C	1.798072	2.875030	-0.853359
C	2.025521	1.516294	2.767731
H	0.938278	1.668136	2.923723
C	2.746686	2.074146	4.000027
H	2.609586	3.170700	4.095066
H	3.837049	1.871113	3.970437
H	2.354795	1.598752	4.922007
C	2.240168	-0.000175	2.626038
H	1.707601	-0.383812	1.731000
H	1.863310	-0.545381	3.515806
H	3.316336	-0.238649	2.499347
C	0.789794	2.954764	-1.993628
H	-0.025997	2.242748	-1.736918
C	1.377166	2.505103	-3.339182
H	1.836643	1.500194	-3.264264
H	2.152073	3.206820	-3.711235
H	0.580319	2.461567	-4.109509
C	0.167960	4.356838	-2.114941
H	-0.333777	4.671370	-1.179395
H	-0.586319	4.382435	-2.928271
H	0.945381	5.114203	-2.348366
C	-1.490589	-1.897959	-0.434465
C	-0.811631	-3.007577	0.150343
C	-0.724310	-4.202473	-0.585229
H	-0.202056	-5.066103	-0.144997
C	-1.277764	-4.313580	-1.866573
H	-1.189035	-5.255621	-2.428228
C	-1.938076	-3.214027	-2.433637
H	-2.366477	-3.304111	-3.443151
C	-2.058022	-1.998081	-1.741992
C	-0.186205	-2.921266	1.538113
H	-0.277289	-1.866259	1.869272
C	1.310594	-3.270084	1.513815
H	1.758104	-3.147069	2.520997
H	1.861174	-2.615170	0.812650
H	1.479222	-4.320880	1.199732
C	-0.933312	-3.805916	2.552076
H	-0.500992	-3.689460	3.567299
H	-0.860219	-4.878770	2.277208
H	-2.010152	-3.551636	2.610330
C	-2.720154	-0.789089	-2.394847
H	-3.025323	-0.099764	-1.580717
C	-1.701060	-0.029859	-3.262775
H	-0.820689	0.269178	-2.655993
H	-2.145002	0.890477	-3.695593
H	-1.333558	-0.666161	-4.094138
C	-3.981378	-1.141345	-3.195125
H	-4.709509	-1.709925	-2.581601
H	-3.749302	-1.751134	-4.092461
H	-4.481312	-0.218017	-3.552135

Conformation 23.
Multiplicity: 4
Charge: 0
E(B97-3c) = -3093.970677203439 Hartree
E(M06/def2-TZVP) = -3093.639284805517 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3092.610637005292 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3092.836393850187 Hartree
E(PBEh-3c) = -3089.875041409444 Hartree
E(PM6) = 9.33738 Kcal/mol
E(PM7) = 12.06737 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3095.695327704533 Hartree
E(GFN1-xTB) = -132.181176917506 Hartree
E(GFN2-xTB) = -130.928819096395 Hartree
E(GFN-FF) = -18.190447927935 Hartree

Coordinates:

Co	0.005793	-0.482125	0.506378
C	-1.132498	-2.122092	0.358039
H	-1.012718	-2.498634	-0.681105
H	-0.599881	-2.858785	1.010866
C	-2.600778	-2.014028	0.757400
H	-2.687087	-1.607029	1.786544
H	-3.111371	-1.261010	0.121187
C	-3.398543	-3.332832	0.701978
H	-4.432429	-3.134405	1.063153
H	-2.960215	-4.054053	1.427138
C	-3.456889	-4.003914	-0.679198
H	-2.447710	-4.389606	-0.941629
H	-4.113529	-4.900034	-0.611394
C	-3.947968	-3.105764	-1.825714
H	-3.973454	-3.708160	-2.759803
H	-3.199462	-2.306525	-2.012278
C	-5.318760	-2.464806	-1.596680
H	-5.658293	-1.904356	-2.491833
H	-5.302156	-1.749349	-0.748614
H	-6.092291	-3.228742	-1.368787
N	-0.390104	1.368448	0.858008
N	1.725770	-0.270607	-0.325131
C	0.170223	3.896082	0.783224
C	0.462696	2.369270	0.571684
C	1.746580	2.100844	0.036424
H	2.366304	2.991013	-0.088187
C	2.366733	0.905771	-0.410517
C	3.832508	1.096577	-0.931721
C	-1.168112	4.245105	1.462668
H	-1.206620	5.344527	1.604324
H	-1.281229	3.775330	2.456227
H	-2.046568	3.956360	0.860945
C	1.288313	4.512013	1.663898
H	1.067536	5.584810	1.839104
H	2.288600	4.454126	1.194366
H	1.348634	4.010622	2.649101
C	0.186609	4.594804	-0.598575
H	0.004161	5.682150	-0.472389
H	-0.605092	4.194559	-1.261276
H	1.156023	4.469020	-1.118472
C	3.884256	2.248834	-1.966541
H	4.918393	2.347099	-2.354685
H	3.600340	3.229320	-1.539697
H	3.216614	2.050672	-2.828404
C	4.475617	-0.130484	-1.607210
H	4.618400	-0.979433	-0.917787
H	5.476023	0.166395	-1.982881
H	3.890261	-0.497816	-2.469076
C	4.708459	1.483655	0.286453
H	4.709648	0.680032	1.048531
H	4.347706	2.410831	0.772625
H	5.757402	1.647520	-0.037010
C	-1.748420	1.428476	1.266293
C	-2.105198	1.172963	2.625343
C	-3.474337	1.155321	2.955113
H	-3.756921	0.970645	4.004193
C	-4.473255	1.355468	1.996086
H	-5.534215	1.329587	2.286245
C	-4.108739	1.583541	0.663415
H	-4.891906	1.731323	-0.095728
C	-2.760124	1.631682	0.275607
C	-1.126776	0.823554	3.752444
H	-1.681922	1.054161	4.688036
C	0.191884	1.606212	3.827089
H	0.029206	2.699536	3.768130
H	0.893091	1.320004	3.020216
H	0.689673	1.396099	4.795887
C	-0.847569	-0.688964	3.765309
H	-1.776666	-1.281766	3.871255
H	-0.154723	-0.963761	4.586699
H	-0.369598	-0.991902	2.806966
C	-2.402496	1.851105	-1.191368
H	-1.321205	2.088113	-1.238756
C	-3.165662	3.023666	-1.826503
H	-3.047899	3.958169	-1.242013
H	-4.251905	2.813162	-1.907075
H	-2.793659	3.213906	-2.853988
C	-2.604818	0.558733	-1.999969
H	-2.012456	-0.267770	-1.561633
H	-2.282146	0.695994	-3.052850
H	-3.670317	0.248947	-2.004218
C	2.123466	-1.568933	-0.735658
C	1.617874	-2.089617	-1.966703
C	1.994291	-3.390219	-2.342889
H	1.628361	-3.800445	-3.295337
C	2.808388	-4.181839	-1.521950
H	3.091775	-5.196808	-1.838910
C	3.229019	-3.688595	-0.280291
H	3.832506	-4.328419	0.381788
C	2.892265	-2.391274	0.140231
C	0.657068	-1.268041	-2.818263
H	0.092935	-0.642709	-2.091233
C	-0.362655	-2.126968	-3.576716
H	-1.146473	-1.482309	-4.022682
H	-0.862242	-2.854630	-2.907098
H	0.106172	-2.692611	-4.408749
C	1.374119	-0.307610	-3.780708
H	0.636691	0.275806	-4.370053
H	2.016672	-0.864976	-4.494171
H	2.012892	0.413977	-3.238612
C	3.290319	-1.904612	1.528343
H	3.128187	-0.807713	1.551647
C	2.357880	-2.521707	2.586419
H	1.299850	-2.284665	2.360156
H	2.587020	-2.130867	3.599484
H	2.457676	-3.626537	2.609205
C	4.765307	-2.165733	1.867493
H	5.444264	-1.737844	1.102641
H	4.985952	-3.250399	1.942754
H	5.023658	-1.711104	2.845964

Conformation 25.
Multiplicity: 4
Charge: 0
E(B97-3c) = -3093.968834915629 Hartree
E(M06/def2-TZVP) = -3093.635385306203 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3092.609478592261 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3092.837790189364 Hartree
E(PBEh-3c) = -3089.873043529812 Hartree
E(PM6) = 10.10311 Kcal/mol
E(PM7) = 10.92971 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3095.697755080522 Hartree
E(GFN1-xTB) = -132.181804772279 Hartree
E(GFN2-xTB) = -130.929993570523 Hartree
E(GFN-FF) = -18.187415100389 Hartree

Coordinates:

Co	0.397977	0.403911	0.146975
C	2.127776	1.149407	0.830571
H	2.989673	0.690199	0.293184
H	2.048021	2.192384	0.442535
C	2.413162	1.164822	2.333128
H	3.268061	1.851719	2.553395
H	1.550685	1.605621	2.883575
C	2.744510	-0.212871	2.913373
H	3.608383	-0.629232	2.349145
H	1.902241	-0.904498	2.709589
C	3.061368	-0.238823	4.412973
H	3.450373	-1.246535	4.680996
H	3.888765	0.474004	4.635760
C	1.867030	0.074355	5.321996
H	1.047013	-0.639740	5.084763
H	1.466875	1.083833	5.082610
C	2.200839	0.000395	6.812207
H	2.570062	-1.008909	7.092031
H	1.318778	0.221542	7.447276
H	2.997068	0.725206	7.083524
N	-0.429092	1.235369	-1.408570
N	-0.329978	-1.389058	-0.045726
C	-2.149271	1.261402	-3.335604
C	-1.329712	0.601010	-2.173507
C	-1.665106	-0.758158	-1.941728
H	-2.421795	-1.142913	-2.629332
C	-1.254591	-1.700684	-0.964956
C	-1.994775	-3.079591	-1.069076
C	-1.885872	2.755004	-3.604036
H	-2.584119	3.088794	-4.398719
H	-0.860666	2.957104	-3.955443
H	-2.060737	3.388669	-2.716618
C	-1.862271	0.497313	-4.650358
H	-2.441674	0.947837	-5.482639
H	-2.139366	-0.572433	-4.586854
H	-0.788120	0.551441	-4.916547
C	-3.654732	1.141728	-2.984043
H	-4.264247	1.620168	-3.778059
H	-3.877630	1.654662	-2.026514
H	-3.990381	0.092166	-2.886857
C	-1.623774	-4.140310	-0.015346
H	-2.211208	-5.056444	-0.229859
H	-1.868477	-3.821475	1.013646
H	-0.556131	-4.417386	-0.033095
C	-1.704864	-3.691615	-2.460914
H	-2.049705	-3.045456	-3.290415
H	-2.218450	-4.670418	-2.557097
H	-0.618626	-3.861999	-2.600427
C	-3.517197	-2.832239	-0.920852
H	-3.925321	-2.175844	-1.712655
H	-3.748700	-2.365653	0.058292
H	-4.057957	-3.799638	-0.971390
C	0.092433	2.546631	-1.540445
C	-0.334533	3.554041	-0.626627

C	0.231413	4.836979	-0.721802
H	-0.108255	5.626943	-0.034136
C	1.222785	5.126095	-1.667695
H	1.652694	6.137070	-1.729532
C	1.682018	4.110069	-2.515735
H	2.486960	4.327678	-3.234926
C	1.144267	2.812669	-2.466378
C	-1.377302	3.255957	0.445598
H	-1.523055	2.153339	0.447358
C	-2.736928	3.901197	0.130098
H	-3.136744	3.560724	-0.845364
H	-2.650883	5.007126	0.088959
H	-3.484366	3.648754	0.910495
C	-0.886775	3.659429	1.845321
H	0.082434	3.179141	2.086004
H	-1.621935	3.360114	2.619974
H	-0.749270	4.756818	1.930398
C	1.729177	1.718337	-3.353890
H	1.089595	0.819584	-3.241024
C	3.142660	1.338768	-2.874519
H	3.140247	1.050070	-1.806902
H	3.842524	2.192485	-2.989191
H	3.543130	0.488362	-3.463974
C	1.752862	2.098470	-4.843834
H	0.748923	2.378967	-5.219486
H	2.118924	1.248099	-5.454895
H	2.431887	2.955104	-5.034421
C	0.179545	-2.174517	1.016564
C	1.395311	-2.905923	0.884500
C	1.864607	-3.605042	2.016831
H	2.805339	-4.172019	1.926578
C	1.191079	-3.584910	3.240790
H	1.589994	-4.139101	4.103328
C	0.018020	-2.826590	3.367345
H	-0.502935	-2.791029	4.335270
C	-0.495578	-2.109523	2.277919
C	2.253863	-3.038034	-0.380666
H	3.297162	-3.022849	0.006523
C	2.176347	-1.918651	-1.425954
H	3.021865	-2.019698	-2.137112
H	2.252390	-0.921974	-0.950834
H	1.239755	-1.944890	-2.015329
C	2.067459	-4.414279	-1.050644
H	2.820638	-4.559322	-1.852314
H	1.066342	-4.500769	-1.518040
H	2.173497	-5.245063	-0.324933
C	-1.729669	-1.227056	2.426485
H	-2.208786	-1.162341	1.428490
C	-2.776409	-1.778503	3.401779
H	-3.068663	-2.815292	3.138765
H	-3.689623	-1.149840	3.382899
H	-2.409819	-1.785122	4.448901
C	-1.315204	0.201286	2.819108
H	-0.542217	0.615599	2.125957
H	-0.854378	0.222178	3.827333
H	-2.178936	0.896108	2.806726

Conformation 28.
Multiplicity: 4
Charge: 0
E(B97-3c) = -3093.960874786102 Hartree
E(M06/def2-TZVP) = -3093.629286916373 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3092.602374126739 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3092.831855513065 Hartree
E(PBEh-3c) = -3089.864124178142 Hartree
E(PM6) = 19.93019 Kcal/mol
E(PM7) = 17.37411 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3095.687345127710 Hartree
E(GFN1-xTB) = -132.170290432317 Hartree
E(GFN2-xTB) = -130.917971488172 Hartree
E(GFN-FF) = -18.174791027163 Hartree

Coordinates:

Co	-0.403057	-0.381328	-0.327386
C	-1.941914	-1.283037	-1.266799
H	-1.975903	-1.001053	-2.344114
H	-1.442320	-2.280742	-1.255541
C	-3.375433	-1.462260	-0.753561
H	-3.802132	-2.373583	-1.236112
H	-3.379966	-1.702778	0.335028
C	-4.341802	-0.296772	-1.018256
H	-5.386417	-0.678370	-1.024029
H	-4.163685	0.082430	-2.047657
C	-4.227313	0.858890	-0.015834
H	-3.152556	1.088937	0.133748
H	-4.669184	1.783334	-0.446966
C	-4.883677	0.588248	1.346066
H	-4.541232	1.363002	2.064724
H	-4.512094	-0.380310	1.749998
C	-6.413707	0.572920	1.315295
H	-6.815639	1.548156	0.967957
H	-6.842230	0.373109	2.318598
H	-6.806971	-0.206196	0.630073
N	1.293255	-1.394358	-0.372616
N	0.333723	1.395484	0.064407
C	3.755927	-1.683452	0.311509
C	2.465901	-0.854704	-0.022513
C	2.589032	0.538139	0.228313
H	3.604847	0.837737	0.471767
C	1.652654	1.596104	0.286956
C	2.238703	3.006668	0.657421
C	3.819515	-3.111686	-0.265701
H	4.784359	-3.565202	0.039939
H	3.775158	-3.125463	-1.368702
H	3.013814	-3.765428	0.104876
C	5.044732	-0.962410	-0.154204
H	5.916263	-1.621788	0.031629
H	5.241370	-0.016255	0.385050
H	5.019208	-0.736456	-1.238284
C	3.786759	-1.790368	1.858375
H	4.679693	-2.364219	2.183221
H	2.888074	-2.313588	2.238976
H	3.823215	-0.789599	2.331728
C	3.784158	3.035185	0.605851
H	4.122057	4.073218	0.796358
H	4.176309	2.728964	-0.383942
H	4.251447	2.398154	1.382488
C	1.837580	3.414346	2.094632
H	0.751312	3.588599	2.195601
H	2.354386	4.358387	2.364683
H	2.140874	2.641712	2.829426
C	1.759095	4.088410	-0.332060
H	0.677242	4.283687	-0.246316
H	1.984480	3.804061	-1.379089
H	2.284731	5.041226	-0.118398
C	1.050665	-2.666372	-0.950401
C	1.150206	-2.811524	-2.367569
C	0.812582	-4.059597	-2.925357
H	0.893380	-4.183226	-4.017456
C	0.357821	-5.126759	-2.141681
H	0.095201	-6.086948	-2.610283
C	0.211058	-4.948075	-0.761493
H	-0.173925	-5.774844	-0.144297
C	0.541066	-3.728501	-0.146634
C	1.590007	-1.715639	-3.346954
H	1.211095	-2.072541	-4.329178
C	3.118356	-1.613354	-3.493027
H	3.579846	-2.602106	-3.688151
H	3.580392	-1.187639	-2.581620
H	3.378383	-0.942174	-4.337550
C	0.981769	-0.317795	-3.144150
H	-0.111264	-0.366567	-2.978528
H	1.148234	0.293370	-4.055424
H	1.442725	0.230185	-2.299231
C	0.331449	-3.563586	1.355093
H	0.712135	-2.556154	1.625621
C	1.114576	-4.602930	2.176043
H	2.196357	-4.590451	1.938364
H	0.742599	-5.630533	1.984493
H	1.002054	-4.407370	3.262270
C	-1.164267	-3.612816	1.713868
H	-1.738857	-2.843770	1.163818
H	-1.316003	-3.445617	2.800183
H	-1.601748	-4.600270	1.460248
C	-0.719652	2.283687	0.411044
C	-1.216277	2.252976	1.751042
C	-2.276292	3.105746	2.099515
H	-2.654993	3.104715	3.132015
C	-2.868115	3.949086	1.148758
H	-3.697252	4.611685	1.438838
C	-2.420175	3.921615	-0.177043
H	-2.912105	4.558956	-0.927204
C	-1.356229	3.092228	-0.575671
C	-0.657370	1.232658	2.737163
H	0.407718	1.067579	2.479451
C	-1.376325	-0.115193	2.553779
H	-0.865077	-0.931740	3.100597
H	-1.446518	-0.414765	1.475437
H	-2.428390	-0.058731	2.898776
C	-0.715153	1.673169	4.203760
H	-0.214491	0.924285	4.850115
H	-1.759035	1.767780	4.567334
H	-0.211752	2.648733	4.356535
C	-0.937985	3.022015	-2.039519
H	0.062663	2.544491	-2.065609
C	-1.899625	2.102180	-2.810397
H	-1.957970	1.109100	-2.327533
H	-1.561198	1.962574	-3.857835
H	-2.924195	2.528599	-2.831807
C	-0.841903	4.394001	-2.722421
H	-0.178133	5.090301	-2.173641
H	-1.837697	4.875473	-2.811093

H	-0.445012	4.282694	-3.752013

Conformation 31.
Multiplicity: 4
Charge: 0
E(B97-3c) = -3093.965455867829 Hartree
E(M06/def2-TZVP) = -3093.629400858030 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3092.606612819721 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3092.833781489612 Hartree
E(PBEh-3c) = -3089.869251266124 Hartree
E(PM6) = 11.83661 Kcal/mol
E(PM7) = 14.50920 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3095.693471187178 Hartree
E(GFN1-xTB) = -132.174847326341 Hartree
E(GFN2-xTB) = -130.923031769479 Hartree
E(GFN-FF) = -18.183856452005 Hartree

Coordinates:

Co	-0.161102	-0.299109	0.415017
C	0.126946	-0.083736	2.369161
H	-0.309662	0.903180	2.639664
H	-0.533083	-0.851001	2.841143
C	1.558166	-0.195536	2.890589
H	2.218256	0.526285	2.356342
H	1.600369	0.107542	3.964374
C	2.147213	-1.601879	2.745313
H	1.995909	-1.926026	1.692476
H	1.552215	-2.314576	3.361404
C	3.634325	-1.728553	3.093492
H	3.980955	-2.758132	2.847632
H	4.216469	-1.047255	2.432343
C	3.986696	-1.431493	4.555311
H	3.381092	-2.090396	5.217546
H	3.681686	-0.392818	4.806999
C	5.473618	-1.612396	4.863119
H	5.805765	-2.651600	4.655473
H	5.707390	-1.392489	5.924578
H	6.096754	-0.939345	4.237137
N	-1.973881	-0.325158	-0.260641
N	0.677060	0.731363	-0.998164
C	-3.726689	0.023674	-2.123729
C	-2.320330	0.194403	-1.447637
C	-1.374568	0.888118	-2.244107
H	-1.784666	1.261664	-3.183351
C	0.007659	1.158780	-2.083118
C	0.636220	1.957332	-3.281392
C	-3.558974	-1.019271	-3.255700
H	-4.521478	-1.161817	-3.789818
H	-3.249833	-2.001558	-2.846627
H	-2.795685	-0.703867	-3.993610
C	-4.874961	-0.453040	-1.210872
H	-5.803835	-0.482681	-1.816457
H	-5.051626	0.236150	-0.364696
H	-4.715313	-1.464489	-0.799463
C	-4.199228	1.366398	-2.736117
H	-5.220787	1.242023	-3.148860
H	-3.558875	1.724443	-3.564307
H	-4.238922	2.165834	-1.969183
C	0.312335	1.228460	-4.612485
H	0.781155	1.778123	-5.453970
H	-0.772162	1.167302	-4.821625
H	0.716192	0.196988	-4.616988
C	2.167432	2.129933	-3.250794
H	2.521778	2.744930	-2.407726
H	2.476561	2.636603	-4.187708
H	2.700592	1.163757	-3.201909
C	-0.009919	3.363567	-3.324215
H	0.188706	3.930390	-2.394742
H	-1.107776	3.307756	-3.455773
H	0.408661	3.944986	-4.171661
C	-2.774219	-1.078769	0.636160
C	-3.533878	-0.465228	1.675559
C	-4.304724	-1.313819	2.499042
H	-4.941228	-0.856134	3.272395
C	-4.298154	-2.704229	2.366220
H	-4.917920	-3.327344	3.028181
C	-3.485378	-3.295704	1.390267
H	-3.453895	-4.391647	1.298038
C	-2.721155	-2.505590	0.520653
C	-3.644894	1.036488	1.997301
H	-4.738481	1.253726	1.964332
C	-2.972167	2.055234	1.067370
H	-3.343461	2.007073	0.028198
H	-1.873593	1.924256	1.031563
H	-3.177789	3.076321	1.448420
C	-3.187519	1.309066	3.447692
H	-3.710762	0.670899	4.185076
H	-3.379531	2.367246	3.718968
H	-2.101544	1.118812	3.553929
C	-1.791844	-3.157902	-0.497084
H	-1.584703	-2.406034	-1.285065
C	-2.393240	-4.390464	-1.184709
H	-3.380042	-4.162542	-1.635915
H	-2.535031	-5.234453	-0.478612
H	-1.721724	-4.751318	-1.990289
C	-0.449507	-3.499209	0.173942
H	-0.007063	-2.605849	0.676277
H	0.291753	-3.879041	-0.558619
H	-0.581702	-4.262188	0.968840
C	2.019513	0.964735	-0.608907
C	2.949872	-0.120582	-0.672892
C	4.262732	0.091331	-0.220276
H	4.992592	-0.728093	-0.277413
C	4.658349	1.322613	0.319821
H	5.690984	1.465656	0.671586
C	3.723187	2.357200	0.434846
H	4.026476	3.312191	0.890886
C	2.399476	2.206004	-0.014649
C	2.500897	-1.488636	-1.180569
H	1.492075	-1.646965	-0.725369
C	3.395361	-2.647238	-0.727217
H	2.921002	-3.616235	-0.982620
H	3.579991	-2.632767	0.363890
H	4.379611	-2.624522	-1.239663
C	2.299540	-1.544886	-2.703281
H	1.943944	-2.550027	-3.010430
H	3.253195	-1.345517	-3.234869
H	1.551529	-0.807612	-3.042806
C	1.407463	3.348526	0.179747
H	0.485409	3.088986	-0.378543
C	1.015455	3.489552	1.661542
H	0.598270	2.545266	2.055772
H	0.254529	4.286792	1.792724
H	1.896863	3.755437	2.281697
C	1.930174	4.691203	-0.360153
H	2.253928	4.621105	-1.417267
H	2.795655	5.055612	0.230356
H	1.140505	5.467452	-0.295744

Conformation 6.
Multiplicity: 4
Charge: 0
E(B97-3c) = -3093.971023226195 Hartree
E(M06/def2-TZVP) = -3093.637498203542 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3092.610163129074 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3092.835533710656 Hartree
E(PBEh-3c) = -3089.876603004644 Hartree
E(PM6) = 8.97611 Kcal/mol
E(PM7) = 11.82756 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3095.698526933079 Hartree
E(GFN1-xTB) = -132.181100983226 Hartree
E(GFN2-xTB) = -130.929081977177 Hartree
E(GFN-FF) = -18.190268496539 Hartree

Coordinates:

Co	-0.408296	-0.002955	-0.174162
C	-2.271400	0.723510	-0.205758
H	-2.314709	1.309244	-1.153393
H	-2.917590	-0.171065	-0.369674
C	-2.766548	1.562341	0.972756
H	-2.836742	0.939160	1.891338
H	-1.996150	2.323043	1.211898
C	-4.099797	2.321318	0.754672
H	-4.136470	2.660848	-0.305674
H	-4.072453	3.253720	1.361314
C	-5.415554	1.604538	1.098311
H	-5.449367	1.413911	2.195589
H	-6.239545	2.324296	0.901223
C	-5.717056	0.285771	0.359152
H	-5.289507	0.332351	-0.666581
H	-6.815497	0.188782	0.219177
C	-5.208890	-0.962630	1.083976
H	-5.716127	-1.084334	2.064379
H	-4.122784	-0.907156	1.288765
H	-5.390970	-1.885748	0.495996
N	0.748911	-0.619021	1.238127
N	0.938765	0.185449	-1.534839
C	2.941057	-1.581122	2.182448
C	2.046916	-0.919307	1.082720
C	2.688214	-0.722291	-0.164632
H	3.738946	-1.022114	-0.179015
C	2.218802	-0.193698	-1.393783
C	3.312190	-0.091690	-2.507608
C	2.312816	-1.690640	3.583697
H	3.032849	-2.213165	4.245946
H	1.372217	-2.267718	3.593611
H	2.104756	-0.703445	4.033181
C	3.258232	-3.019143	1.702133
H	3.896275	-3.537373	2.447824
H	3.789152	-3.026261	0.730542
H	2.326758	-3.608646	1.581233
C	4.256090	-0.783055	2.347222

H	4.882318	-1.255685	3.131259
H	4.048451	0.259665	2.662638
H	4.859424	-0.741753	1.420456
C	2.839242	0.413801	-3.882969
H	3.718016	0.442802	-4.559169
H	2.408629	1.429478	-3.850867
H	2.086140	-0.250819	-4.341817
C	3.918489	-1.498001	-2.740955
H	4.416649	-1.907317	-1.841500
H	4.676103	-1.448288	-3.549813
H	3.135438	-2.219015	-3.051637
C	4.412089	0.876502	-2.008320
H	4.880579	0.528902	-1.067744
H	3.992564	1.885372	-1.821525
H	5.209958	0.973865	-2.773506
C	-0.075079	-0.587991	2.388896
C	-0.039885	0.547963	3.254874
C	-1.010074	0.641557	4.264655
H	-1.005989	1.511402	4.938026
C	-1.990438	-0.349213	4.429391
H	-2.751249	-0.245624	5.217489
C	-1.987498	-1.477505	3.599372
H	-2.743054	-2.264219	3.751464
C	-1.031806	-1.628228	2.579165
C	1.025659	1.623185	3.065738
H	1.906674	1.123235	2.613182
C	1.491426	2.258881	4.381756
H	1.798844	1.492254	5.121877
H	0.696862	2.877591	4.847486
H	2.357022	2.927697	4.199675
C	0.573219	2.692820	2.059942
H	0.238929	2.222068	1.113484
H	1.399013	3.395454	1.824554
H	-0.277874	3.280257	2.461091
C	-0.984274	-2.902146	1.741090
H	-0.157019	-2.778310	1.011132
C	-2.272571	-3.130494	0.938534
H	-2.492816	-2.261052	0.291136
H	-3.147336	-3.283429	1.602961
H	-2.179006	-4.026912	0.291841
C	-0.659020	-4.131128	2.609452
H	0.281180	-3.996004	3.180008
H	-0.547886	-5.036830	1.978155
H	-1.467153	-4.331729	3.343041
C	0.259547	0.704942	-2.667705
C	0.094532	2.113184	-2.811550
C	-0.673072	2.590286	-3.888235
H	-0.800794	3.676641	-4.015316
C	-1.283300	1.713842	-4.794325
H	-1.882160	2.108564	-5.628855
C	-1.138160	0.330193	-4.624248
H	-1.631530	-0.356520	-5.329317
C	-0.374979	-0.199220	-3.570885
C	0.712498	3.094827	-1.822567
H	1.210676	2.491719	-1.036228
C	-0.365766	3.951032	-1.137012
H	0.084932	4.592756	-0.352822
H	-1.136676	3.316568	-0.660219
H	-0.876120	4.617186	-1.863128
C	1.779405	3.987582	-2.480276
H	2.238545	4.664628	-1.730621
H	1.338498	4.621304	-3.277621
H	2.591672	3.391130	-2.940859
C	-0.269540	-1.707500	-3.374329
H	0.544213	-1.889066	-2.642953
C	-1.567208	-2.253091	-2.753210
H	-1.794418	-1.733105	-1.800500
H	-1.485707	-3.338737	-2.538928
H	-2.430812	-2.096669	-3.432237
C	0.087773	-2.462044	-4.663761
H	1.019204	-2.073175	-5.122820
H	-0.717391	-2.385245	-5.423297
H	0.235760	-3.540776	-4.452285

Conformation 9.
Multiplicity: 4
Charge: 0
E(B97-3c) = -3093.963856053141 Hartree
E(M06/def2-TZVP) = -3093.631833698390 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3092.605265298622 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3092.834249570261 Hartree
E(PBEh-3c) = -3089.869321068853 Hartree
E(PM6) = 14.47656 Kcal/mol
E(PM7) = 14.89500 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3095.692909302862 Hartree
E(GFN1-xTB) = -132.173137986320 Hartree
E(GFN2-xTB) = -130.921770408595 Hartree
E(GFN-FF) = -18.182008739047 Hartree

Coordinates:

Co	0.052541	-0.541344	0.230928
C	-0.450716	-2.101897	1.384869
H	-1.509704	-2.388326	1.191987
H	0.172336	-2.897687	0.910662
C	-0.220410	-2.085951	2.898597
H	-0.313829	-3.127619	3.295970
H	0.827038	-1.788610	3.135318
C	-1.197806	-1.195625	3.672960
H	-2.223964	-1.384361	3.287067
H	-0.997121	-0.130003	3.438874
C	-1.208776	-1.416127	5.192366
H	-2.017544	-0.794177	5.637999
H	-1.491444	-2.473291	5.395931
C	0.106189	-1.108905	5.925126
H	0.926281	-1.724731	5.494327
H	0.012073	-1.441184	6.981949
C	0.504708	0.367534	5.896556
H	0.643301	0.732138	4.859398
H	1.450111	0.549194	6.447451
H	-0.281340	1.004028	6.355046
N	0.781765	-0.823773	-1.558464
N	-0.765378	1.209513	-0.008007
C	1.552226	0.054057	-3.835586
C	0.768575	0.163409	-2.481186
C	0.098406	1.387258	-2.246448
H	0.154228	2.084550	-3.079736
C	-0.606782	1.918131	-1.132376
C	-1.139834	3.375204	-1.370696
C	1.470846	1.342232	-4.684047
H	2.067662	1.191356	-5.605718
H	1.890302	2.223269	-4.159597
H	0.435246	1.577625	-5.000264
C	3.047948	-0.190608	-3.544890
H	3.622175	-0.149203	-4.493109
H	3.222705	-1.182965	-3.094654
H	3.456463	0.583409	-2.864633
C	1.012088	-1.086801	-4.720335
H	1.534504	-1.074302	-5.699116
H	-0.071962	-0.964308	-4.913038
H	1.181071	-2.077970	-4.266113
C	-1.871205	4.047673	-0.193555
H	-2.211764	5.048695	-0.528826
H	-1.219537	4.194214	0.685867
H	-2.760330	3.487966	0.141050
C	-2.126860	3.339316	-2.563150
H	-1.652695	2.975177	-3.494429
H	-2.521028	4.358137	-2.757391
H	-2.988741	2.676954	-2.345476
C	0.059995	4.292631	-1.719905
H	0.587877	3.980302	-2.640509
H	0.799156	4.306517	-0.893226
H	-0.296877	5.332081	-1.871607
C	1.318316	-2.137691	-1.678680
C	0.525074	-3.189972	-2.238419
C	1.056644	-4.491466	-2.273406
H	0.453365	-5.301238	-2.711153
C	2.323157	-4.783253	-1.754102
H	2.719006	-5.809045	-1.797147
C	3.068255	-3.761545	-1.156404
H	4.049948	-3.993630	-0.715695
C	2.587778	-2.441302	-1.095575
C	-0.909078	-2.967813	-2.716274
H	-1.065816	-1.874130	-2.811002
C	-1.899701	-3.491643	-1.660128
H	-1.716852	-3.034353	-0.672766
H	-1.799206	-4.590638	-1.542726
H	-2.945709	-3.272885	-1.958111
C	-1.220565	-3.624141	-4.072428
H	-0.502056	-3.334820	-4.862228
H	-2.236494	-3.335017	-4.410835
H	-1.210387	-4.731111	-3.997818
C	3.397415	-1.395989	-0.332455
H	2.946005	-0.404846	-0.548886
C	4.879325	-1.342870	-0.737889
H	5.010272	-1.193899	-1.826636
H	5.412452	-2.274987	-0.458801
H	5.390243	-0.508849	-0.214529
C	3.274691	-1.655427	1.180390
H	2.215525	-1.648284	1.503005
H	3.819951	-0.887831	1.766271
H	3.692576	-2.648943	1.442610
C	-1.360572	1.610422	1.214818
C	-2.701852	1.261939	1.540585
C	-3.181598	1.634427	2.814858
H	-4.214751	1.361604	3.084566
C	-2.392712	2.320796	3.740264
H	-2.800941	2.591148	4.725452
C	-1.067897	2.643269	3.410867
H	-0.440485	3.172349	4.142560
C	-0.531529	2.288203	2.166542
C	-3.720015	0.557437	0.632016
H	-4.245111	-0.146675	1.316140

C	-3.201197	-0.293608	-0.531869
H	-4.038457	-0.891797	-0.946485
H	-2.418367	-0.999909	-0.199056
H	-2.781758	0.311655	-1.358020
C	-4.791084	1.547869	0.129595
H	-5.598776	1.005662	-0.403794
H	-4.358498	2.282554	-0.578776
H	-5.252892	2.113821	0.966242
C	0.924087	2.578175	1.819432
H	0.974788	2.724518	0.721403
C	1.487814	3.844461	2.473854
H	0.857698	4.730617	2.256509
H	2.509474	4.048877	2.094578
H	1.565484	3.745147	3.576084
C	1.799097	1.356831	2.144979
H	1.343230	0.416823	1.753503
H	1.895683	1.210620	3.240068
H	2.814838	1.447579	1.710688

AJOMIX

Conformation 11.
Multiplicity: 4
Charge: 0
E(B97-3c) = -4478.406797519745 Hartree
E(M06/def2-TZVP) = -4478.394981553469 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -4476.712739708432 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -4477.086899115723 Hartree
E(PBEh-3c) = -4473.003954433887 Hartree
E(PM6) = -142.60181 Kcal/mol
E(PM7) = -204.38983 Kcal/mol
E(ωB97X-V/def2-TZVP) = -4480.434995379660 Hartree
E(GFN1-xTB) = -139.771656147191 Hartree
E(GFN2-xTB) = -136.960811665688 Hartree
E(GFN-FF) = -18.059600203140 Hartree

Coordinates:

C	0.943747	0.175276	-0.817298
C	2.594591	1.031047	-2.166228
H	3.115699	1.809692	-2.728987
C	2.815587	-0.311402	-2.063730
H	3.592034	-0.935453	-2.511222
C	1.021096	2.674169	-1.238478
C	-0.021798	3.163833	-2.068209
C	-0.318405	4.536233	-1.969508
H	-1.121488	4.958629	-2.587063
C	0.374118	5.373387	-1.086604
H	0.111642	6.440470	-1.027103
C	1.385670	4.857950	-0.271086
H	1.915072	5.522189	0.426967
C	1.742036	3.497296	-0.334774
C	-0.803217	2.247123	-3.008328
H	-1.078792	1.357157	-2.399013
C	-2.113876	2.868423	-3.502773
H	-2.767996	3.182206	-2.667436
H	-2.676303	2.127836	-4.103180
H	-1.934834	3.747112	-4.157147
C	0.026982	1.788456	-4.223335
H	0.334453	2.657737	-4.841954
H	-0.581022	1.117753	-4.864393
H	0.940151	1.232879	-3.940546
C	2.902337	2.967650	0.506862
H	2.775809	1.867486	0.591926
C	4.254460	3.243352	-0.181672
H	4.318654	2.787290	-1.186841
H	5.089215	2.839140	0.426842
H	4.414056	4.335456	-0.295974
C	2.932912	3.540644	1.932108
H	3.197074	4.618079	1.934126
H	3.702703	3.016978	2.533440
H	1.962317	3.423284	2.445660
C	3.104887	-2.625191	0.525321
C	2.737363	-1.575878	1.588576
H	1.666392	-1.596454	1.873824
H	2.949094	-0.551654	1.222519
H	3.349939	-1.736979	2.500155
C	4.531219	-2.333884	0.037795
H	5.203552	-2.294915	0.922222
H	4.605588	-1.346375	-0.458650
H	4.932112	-3.105193	-0.642312
C	3.020922	-4.037190	1.137210
H	3.717671	-4.108811	1.999224
H	3.308540	-4.826964	0.413911
H	2.001425	-4.262236	1.512043
C	2.003317	-3.557839	-2.286237
C	3.464639	-3.866442	-2.639702
H	3.488049	-4.470432	-3.572660
H	3.971584	-4.460650	-1.855734
H	4.068478	-2.957520	-2.827779
C	1.268405	-4.884208	-1.981677
H	1.359017	-5.569798	-2.851144
H	0.191083	-4.713496	-1.786074
H	1.694041	-5.404845	-1.100432
C	1.317436	-2.883796	-3.488030
H	1.834000	-1.958575	-3.808641
H	0.263667	-2.630472	-3.271811
H	1.327154	-3.587735	-4.347281
C	-2.732690	3.476409	0.270000
H	-1.630877	3.475242	0.341960
H	-3.129857	4.091884	1.104076
H	-2.999534	3.993604	-0.673920
C	-3.961591	1.237999	2.075318
H	-4.743898	0.451769	2.050513
H	-4.349919	2.087316	2.674609
H	-3.083121	0.801953	2.587053
C	-5.167617	1.970265	-0.610149
H	-5.026216	2.307995	-1.656844
H	-5.741391	2.758962	-0.078403
H	-5.795741	1.056795	-0.623077
C	-4.414872	-1.823432	-0.298907
H	-3.984563	-2.115618	0.678624
H	-4.728628	-2.745657	-0.831213
H	-5.327926	-1.227194	-0.094628
C	-1.746221	-1.915300	-1.906341
H	-1.164993	-1.345324	-2.659443
H	-2.121237	-2.843097	-2.386731
H	-1.047557	-2.217030	-1.099269
C	-4.058704	-0.337756	-2.942279
H	-4.935189	0.319770	-2.789732
H	-4.413424	-1.266013	-3.438789
H	-3.364205	0.170815	-3.640889
C	1.620274	0.544057	3.851634
H	1.883484	-0.445427	4.275127
H	1.819286	1.312059	4.628542
H	2.297917	0.743861	2.999303
C	-1.212803	0.631477	4.941081
H	-2.296215	0.760255	4.746667
H	-0.878763	1.477832	5.577733
H	-1.077927	-0.299813	5.526669
C	-0.463819	2.342764	2.551843
H	-0.014221	2.433280	1.540561
H	-0.005860	3.126514	3.190290
H	-1.540249	2.575917	2.467337
C	-2.962656	-2.116782	3.539309
H	-2.988035	-1.510090	4.465090
H	-3.291363	-3.145820	3.796710
H	-3.705120	-1.686868	2.837929
C	-1.334707	-3.493241	1.391832
H	-2.123028	-3.275594	0.646208
H	-1.584527	-4.464837	1.867508
H	-0.376109	-3.600207	0.848374
C	-0.040746	-2.874219	4.066040
H	0.975285	-3.031175	3.649421
H	-0.411467	-3.853192	4.435937
H	0.057493	-2.203470	4.943575
N	1.468016	1.310531	-1.396567
N	1.808052	-0.824228	-1.249366
N	-2.468070	0.515057	-0.424473
N	-0.676794	-0.607598	2.170342
Si	-3.508164	1.738098	0.299226
Si	-3.174895	-0.813254	-1.325253
Si	-0.205973	0.634180	3.325519
Si	-1.233710	-2.174440	2.749986
P	1.636939	-2.525314	-0.698943
Co	-0.745807	0.023505	0.343588

Conformation 14.
Multiplicity: 4
Charge: 0
E(B97-3c) = -4478.405838585287 Hartree
E(M06/def2-TZVP) = -4478.396031220862 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -4476.710650425274 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -4477.086317034547 Hartree
E(PBEh-3c) = -4473.006022444982 Hartree
E(PM6) = -138.89991 Kcal/mol
E(PM7) = -194.58364 Kcal/mol
E(ωB97X-V/def2-TZVP) = -4480.434159702331 Hartree
E(GFN1-xTB) = -139.767273729267 Hartree
E(GFN2-xTB) = -136.959005112215 Hartree
E(GFN-FF) = -18.067452078324 Hartree

Coordinates:

C	1.087327	0.362499	0.462283
C	3.173120	0.871323	1.273038
H	4.249539	0.736986	1.410510
C	2.305829	1.793180	1.789036
H	2.484308	2.627119	2.471304
C	3.091062	-0.887147	-0.452860
C	3.060747	-2.279277	-0.200288
C	3.743181	-3.117902	-1.101165
H	3.726074	-4.204437	-0.939066

C	4.449163	-2.594240	-2.190222
H	4.978487	-3.270569	-2.878395
C	4.478302	-1.213692	-2.407334
H	5.025743	-0.808966	-3.271096
C	3.791961	-0.329368	-1.554249
C	2.383233	-2.842513	1.036949
H	1.485292	-2.222164	1.233310
C	1.886186	-4.279503	0.861599
H	1.263353	-4.382537	-0.048473
H	1.259224	-4.565138	1.728667
H	2.719289	-5.010529	0.801120
C	3.345254	-2.740481	2.236459
H	4.282068	-3.298927	2.030765
H	2.885398	-3.171755	3.148457
H	3.615392	-1.690362	2.464607
C	3.812526	1.166921	-1.850168
H	3.011480	1.638756	-1.245219
C	5.152560	1.803888	-1.438829
H	5.375160	1.654909	-0.364408
H	5.143135	2.895452	-1.636487
H	5.989850	1.361856	-2.017593
C	3.507251	1.470581	-3.326515
H	4.345813	1.171641	-3.988241
H	3.349739	2.558755	-3.469557
H	2.597810	0.944811	-3.670559
C	-0.081243	3.782873	0.074665
C	1.212597	4.589319	0.255970
H	2.099980	3.930626	0.339896
H	1.193725	5.268867	1.125542
H	1.365890	5.217604	-0.648061
C	-1.308523	4.714011	0.048670
H	-1.229690	5.400403	-0.820891
H	-1.382977	5.343661	0.957702
H	-2.255088	4.146009	-0.062909
C	0.011391	3.026261	-1.261588
H	-0.005054	3.755119	-2.099122
H	-0.805386	2.294339	-1.412934
H	0.957608	2.454872	-1.335422
C	-0.509066	3.171956	3.126313
C	0.333011	4.424980	3.407346
H	0.208562	4.704311	4.475885
H	0.008889	5.295260	2.805659
H	1.416429	4.272850	3.236500
C	-2.002857	3.515176	3.336976
H	-2.149096	3.890026	4.372344
H	-2.649207	2.625588	3.203163
H	-2.357935	4.303544	2.645047
C	-0.125127	2.061789	4.118789
H	0.951062	1.807048	4.082820
H	-0.697519	1.135146	3.941008
H	-0.354203	2.407046	5.149473
C	0.747814	-1.470760	-3.084774
H	1.497536	-1.011705	-2.414423
H	1.242828	-1.645473	-4.063008
H	0.477829	-2.457858	-2.663365
C	-0.157964	1.238124	-4.161400
H	-0.994505	1.932927	-4.372206
H	0.324671	0.987142	-5.129770
H	0.582510	1.780971	-3.545936
C	-1.868084	-1.190371	-4.640430
H	-2.317918	-2.136080	-4.279670
H	-1.246502	-1.425031	-5.530306
H	-2.689280	-0.524898	-4.976426
C	-3.450443	2.070514	-2.858353
H	-2.772551	2.895198	-2.557945
H	-4.494569	2.439586	-2.777207
H	-3.259425	1.847819	-3.928041
C	-3.779384	0.999856	-0.019438
H	-3.780854	0.118869	0.649463
H	-4.810109	1.410045	-0.050151
H	-3.107357	1.756375	0.431363
C	-4.494322	-0.746180	-2.405425
H	-4.414465	-0.895002	-3.499638
H	-5.522991	-0.389054	-2.186973
H	-4.369526	-1.733755	-1.920849
C	0.329786	-1.317765	3.502427
H	0.967533	-2.222397	3.535375
H	0.167829	-0.998071	4.552838
H	0.894455	-0.520612	2.985810
C	-1.896883	-3.252335	3.749064
H	-2.897223	-3.639582	3.472429
H	-1.950549	-2.917407	4.806884
H	-1.173971	-4.091080	3.700553
C	-2.609471	-0.407641	3.086249
H	-2.415207	0.512985	2.503427
H	-2.617790	-0.154759	4.167164
H	-3.624751	-0.762285	2.815460
C	-1.886362	-3.531750	-1.588206
H	-2.026537	-2.565719	-2.104559
H	-2.603818	-4.267784	-2.006451
H	-0.863162	-3.901589	-1.805130
C	-1.780140	-5.113677	0.937818
H	-0.721614	-5.394807	0.774011
H	-2.406250	-5.830687	0.364906
H	-2.012468	-5.250069	2.009760
C	-4.014226	-3.077253	0.593394
H	-4.254072	-3.167761	1.672791
H	-4.632898	-3.823264	0.051745
H	-4.331867	-2.068451	0.265075
N	2.429132	0.030140	0.448328
N	1.046708	1.481135	1.283346
N	-1.572242	-0.074906	-1.782031
N	-1.197651	-2.056844	0.972337
Si	-0.767433	-0.361382	-3.324986
Si	-3.230163	0.523704	-1.764293
Si	-1.335502	-1.761995	2.702408
Si	-2.158923	-3.367741	0.274024
P	-0.487044	2.415471	1.357640
Co	-0.611193	-0.602940	-0.184923

Conformation 17.
Multiplicity: 4
Charge: 0
E(B97-3c) = -4478.404657737991 Hartree
E(M06/def2-TZVP) = -4478.392774683970 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -4476.711087665895 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -4477.084918833831 Hartree
E(PBEh-3c) = -4473.001951029328 Hartree
E(PM6) = -145.17434 Kcal/mol
E(PM7) = -217.64925 Kcal/mol
E(ωB97X-V/def2-TZVP) = -4480.431554094200 Hartree
E(GFN1-xTB) = -139.774184918721 Hartree
E(GFN2-xTB) = -136.959622895509 Hartree
E(GFN-FF) = -18.059908717412 Hartree

Coordinates:

C	-0.207602	-0.900670	-0.728243
C	-1.153471	-2.584555	-1.969549
H	-1.914534	-3.050961	-2.601454
C	0.023504	-3.064460	-1.471157
H	0.494433	-4.041098	-1.596098
C	-2.323705	-0.413657	-2.022173
C	-3.637134	-0.606592	-1.533217
C	-4.659439	0.194362	-2.078274
H	-5.689362	0.074576	-1.710410
C	-4.383395	1.142748	-3.065571
H	-5.192835	1.771182	-3.466530
C	-3.078998	1.290633	-3.555938
H	-2.880922	2.027259	-4.345880
C	-2.020363	0.505262	-3.065361
C	-3.979101	-1.682361	-0.510368
H	-3.028781	-2.094646	-0.121374
C	-4.750495	-1.133817	0.698030
H	-4.139825	-0.393950	1.247135
H	-5.003850	-1.957032	1.396329
H	-5.703513	-0.650272	0.400840
C	-4.752264	-2.832477	-1.183119
H	-5.737052	-2.486882	-1.560343
H	-4.935613	-3.653089	-0.459916
H	-4.199730	-3.254961	-2.046739
C	-0.621956	0.597480	-3.676267
H	0.098939	0.567677	-2.830820
C	-0.323546	-0.612473	-4.585575
H	-0.414628	-1.578377	-4.055029
H	0.710234	-0.545356	-4.982122
H	-1.019420	-0.630827	-5.449718
C	-0.366936	1.888760	-4.461788
H	-0.975976	1.928646	-5.388517
H	0.696232	1.936595	-4.768923
H	-0.582781	2.791937	-3.862543
C	3.291293	-1.655689	-1.513934
C	2.989729	-2.515423	-2.748763
H	1.944969	-2.381855	-3.091775
H	3.172445	-3.593496	-2.588638
H	3.647349	-2.188970	-3.583328
C	4.762190	-1.805844	-1.083580
H	5.418540	-1.412666	-1.888518
H	5.050779	-2.861008	-0.909121
H	4.983256	-1.225882	-0.164246
C	3.018889	-0.180434	-1.861357
H	3.703088	0.144112	-2.674057
H	3.148475	0.495496	-0.994365
H	1.981142	-0.036441	-2.219941
C	2.487327	-3.744619	0.696421
C	2.895046	-4.847080	-0.291676
H	3.032464	-5.798087	0.267143
H	3.852776	-4.628461	-0.801433
H	2.131607	-5.042335	-1.069339
C	3.613298	-3.560040	1.741942
H	3.796755	-4.526618	2.257500
H	3.332109	-2.811373	2.509018
H	4.569151	-3.238278	1.285588

C	1.208400	-4.158622	1.447976
H	0.354885	-4.357721	0.772677
H	0.891483	-3.384341	2.170209
H	1.411091	-5.089490	2.019258
C	-3.492461	2.290662	0.539345
H	-3.002273	1.976717	-0.399103
H	-3.751392	3.365981	0.443193
H	-4.445481	1.730795	0.614215
C	-1.469591	3.589981	2.502861
H	-1.133755	3.574146	3.559558
H	-2.082028	4.502368	2.348452
H	-0.560715	3.653506	1.874948
C	-3.743020	1.827571	3.481930
H	-4.327180	0.888619	3.394835
H	-4.456424	2.672899	3.377798
H	-3.312102	1.874379	4.500167
C	-1.806946	-0.455497	4.805602
H	-1.468259	0.492321	5.271355
H	-1.437947	-1.290539	5.438321
H	-2.913274	-0.476674	4.830693
C	0.770487	-0.964634	3.354403
H	1.329982	-1.076713	2.403442
H	0.922424	-1.888330	3.951987
H	1.224430	-0.122552	3.911088
C	-1.791534	-2.310719	2.392618
H	-2.897278	-2.271255	2.350964
H	-1.509648	-3.163156	3.045413
H	-1.415201	-2.520996	1.371639
C	1.301490	5.124980	0.044898
H	0.883550	5.256124	1.063674
H	0.737565	5.797472	-0.636117
H	2.354212	5.466675	0.054381
C	-0.696607	3.233548	-1.149796
H	-1.041389	2.203824	-1.377719
H	-0.855142	3.843292	-2.063184
H	-1.359332	3.642284	-0.365072
C	2.228299	3.198019	-2.119685
H	3.299518	3.218890	-1.831980
H	2.046006	4.045013	-2.814168
H	2.047784	2.257176	-2.674144
C	3.898013	3.592178	1.490570
H	4.310335	3.546836	0.461326
H	4.747312	3.461965	2.193960
H	3.483020	4.605048	1.652460
C	1.826703	2.595582	3.503665
H	1.511972	3.658501	3.534450
H	2.520365	2.415906	4.351004
H	0.916085	1.982278	3.648194
C	3.744218	0.674769	2.011038
H	3.191802	-0.264378	2.187471
H	4.439735	0.837940	2.861128
H	4.358581	0.543271	1.096190
N	-1.267397	-1.266015	-1.533138
N	0.593847	-2.034100	-0.726779
N	-1.333345	0.647321	1.938754
N	1.403702	2.054198	0.574614
Si	-2.439161	2.007643	2.105164
Si	-1.083018	-0.675158	3.061897
Si	1.110404	3.336862	-0.586631
Si	2.630870	2.205401	1.827417
P	2.215001	-1.957113	0.044032
Co	0.009534	0.701451	0.533429

Conformation 18.
Multiplicity: 4
Charge: 0
E(B97-3c) = -4478.408571759936 Hartree
E(M06/def2-TZVP) = -4478.395992495817 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -4476.715088167532 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -4477.088251999112 Hartree
E(PBEh-3c) = -4473.000947919019 Hartree
E(PM6) = -146.03076 Kcal/mol
E(PM7) = -212.78351 Kcal/mol
E(ωB97X-V/def2-TZVP) = -4480.435841460176 Hartree
E(GFN1-xTB) = -139.774287927001 Hartree
E(GFN2-xTB) = -136.962548868099 Hartree
E(GFN-FF) = -18.048705138171 Hartree

Coordinates:

C	1.120977	-0.474054	0.087169
C	3.169215	-1.455202	-0.250811
H	4.026360	-1.794648	-0.838117
C	2.936485	-1.463208	1.091541
H	3.561207	-1.821921	1.909420
C	2.081782	-0.602292	-2.270789
C	1.896528	-1.688369	-3.161072
C	2.078096	-1.442138	-4.536702
H	1.929339	-2.263356	-5.252705
C	2.445217	-0.176732	-5.000862
H	2.585563	-0.004640	-6.078644
C	2.629466	0.877255	-4.096731
H	2.920131	1.866444	-4.475372
C	2.452762	0.694406	-2.713606
C	1.557691	-3.097107	-2.686034
H	1.192700	-3.019126	-1.642402
C	0.442146	-3.745830	-3.522727
H	-0.437017	-3.081941	-3.619593
H	0.111299	-4.691291	-3.048215
H	0.793526	-3.998229	-4.544435
C	2.807316	-3.999128	-2.689548
H	3.222405	-4.089861	-3.714721
H	2.551064	-5.018761	-2.335784
H	3.611926	-3.608547	-2.036992
C	2.696595	1.833042	-1.728547
H	1.919041	1.733957	-0.943013
C	4.085735	1.725533	-1.069103
H	4.227074	0.774298	-0.522210
H	4.232384	2.552747	-0.344603
H	4.886106	1.799873	-1.834537
C	2.529733	3.218276	-2.359645
H	3.348756	3.451528	-3.071412
H	2.554791	3.997710	-1.572218
H	1.567009	3.301935	-2.895506
C	2.314418	0.527807	3.730533
C	2.813886	1.541184	2.684215
H	1.974568	2.060809	2.181699
H	3.436713	1.065745	1.901632
H	3.434427	2.311897	3.188735
C	3.507703	-0.208804	4.354292
H	4.186612	0.534610	4.825830
H	4.111378	-0.761336	3.608609
H	3.199081	-0.915817	5.148263
C	1.562481	1.300334	4.838310
H	2.260344	2.007050	5.335631
H	1.153730	0.630309	5.620192
H	0.720428	1.889235	4.422611
C	0.805882	-2.246017	3.635651
C	2.024506	-3.181086	3.605258
H	1.757836	-4.119692	4.137926
H	2.916084	-2.764265	4.108097
H	2.295854	-3.472055	2.572918
C	0.360222	-2.036617	5.096359
H	0.020322	-3.005091	5.520267
H	-0.485467	-1.325169	5.181679
H	1.187485	-1.668073	5.734981
C	-0.326121	-2.908882	2.825574
H	0.000507	-3.115878	1.787039
H	-1.226928	-2.272362	2.763298
H	-0.603038	-3.877889	3.293151
C	-0.020521	3.149536	0.737770
H	-0.050806	2.170543	1.267010
H	-0.238921	3.930497	1.494170
H	1.015721	3.299059	0.372689
C	-3.011357	3.471171	-0.149450
H	-3.639475	3.808477	-0.998125
H	-3.080550	4.241901	0.646108
H	-3.443583	2.528346	0.232042
C	-0.823640	4.770438	-1.735358
H	0.207845	4.790955	-2.134280
H	-0.950888	5.650566	-1.069520
H	-1.527295	4.896878	-2.583161
C	-3.410995	2.121479	-3.413294
H	-4.106085	1.709994	-2.654794
H	-3.802530	1.854717	-4.417589
H	-3.441953	3.227615	-3.329425
C	-1.569847	-0.321771	-3.800204
H	-0.544463	-0.728461	-3.701433
H	-1.842570	-0.357429	-4.875484
H	-2.268115	-0.981252	-3.251554
C	-0.612157	2.456257	-4.490508
H	-0.547586	3.533532	-4.242757
H	-1.095257	2.367497	-5.486598
H	0.415177	2.054112	-4.577440
C	-2.264638	1.944481	3.012547
H	-1.211556	1.740397	3.290202
H	-2.816705	2.216855	3.936285
H	-2.288463	2.813537	2.332234
C	-3.172060	-0.787256	3.795515
H	-3.549432	-1.797050	3.546092
H	-3.866584	-0.341075	4.538503
H	-2.187703	-0.898875	4.289708
C	-4.883461	0.768358	1.875873
H	-4.999549	1.391993	0.967630
H	-5.358738	1.308132	2.722046
H	-5.459022	-0.167139	1.716348
C	-4.253860	-1.048239	-1.207385
H	-5.167470	-0.720367	-0.672159
H	-4.541573	-1.861039	-1.906763
H	-3.891589	-0.189727	-1.803442
C	-1.519574	-2.466237	-0.937459
H	-0.911916	-1.740966	-1.519525
H	-1.910820	-3.212274	-1.658651

H	-0.837417	-2.985006	-0.234237
C	-3.746167	-2.985028	1.071809
H	-3.046454	-3.429495	1.807099
H	-4.095768	-3.796690	0.399088
H	-4.631879	-2.607915	1.622047
N	2.060866	-0.857227	-0.849539
N	1.689490	-0.868669	1.289338
N	-1.026958	1.667699	-1.570719
N	-2.202897	-0.305404	0.920965
Si	-1.226470	3.201670	-0.736659
Si	-1.626923	1.477044	-3.211683
Si	-3.061158	0.383040	2.291406
Si	-2.928147	-1.625560	0.020251
P	0.921404	-0.489597	2.870652
Co	-0.733281	0.342398	-0.180458

Conformation 19.
Multiplicity: 4
Charge: 0
E(B97-3c) = -4478.408422031329 Hartree
E(M06/def2-TZVP) = -4478.398017093015 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -4476.714887455842 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -4477.089377533198 Hartree
E(PBEh-3c) = -4473.006910938894 Hartree
E(PM6) = -144.35197 Kcal/mol
E(PM7) = -214.56319 Kcal/mol
E(ωB97X-V/def2-TZVP) = -4480.436973878229 Hartree
E(GFN1-xTB) = -139.773431813220 Hartree
E(GFN2-xTB) = -136.962891733865 Hartree
E(GFN-FF) = -18.064249752487 Hartree

Coordinates:

C	1.080817	-0.624478	-0.110882
C	2.912550	-1.867421	-0.712386
H	3.647162	-2.291812	-1.401995
C	2.804687	-1.942045	0.646643
H	3.435770	-2.451754	1.377361
C	1.795303	-0.644619	-2.541570
C	1.466094	-1.594920	-3.540038
C	1.490949	-1.167769	-4.882844
H	1.230959	-1.882922	-5.676648
C	1.823588	0.146230	-5.218392
H	1.823160	0.463566	-6.272044
C	2.162057	1.061030	-4.213462
H	2.439161	2.086890	-4.490444
C	2.172683	0.688647	-2.857437
C	1.112117	-3.044194	-3.228305
H	0.903682	-3.114975	-2.142336
C	-0.153754	-3.501343	-3.973752
H	-0.984250	-2.782007	-3.844065
H	-0.488310	-4.487101	-3.592967
H	0.032115	-3.615422	-5.061478
C	2.288094	-3.984792	-3.553622
H	2.537958	-3.943340	-4.633985
H	2.027499	-5.034161	-3.306113
H	3.206997	-3.723202	-2.992394
C	2.659245	1.658322	-1.786579
H	2.008665	1.509218	-0.900260
C	4.117254	1.341732	-1.399282
H	4.241581	0.303828	-1.035548
H	4.462019	2.023906	-0.595805
H	4.787086	1.478245	-2.273512
C	2.531336	3.126805	-2.195460
H	3.244310	3.400624	-3.000681
H	2.754408	3.781820	-1.330228
H	1.505369	3.353491	-2.537925
C	2.761164	0.212952	3.306174
C	3.387407	0.996080	2.139705
H	2.634507	1.582217	1.578916
H	3.907749	0.329351	1.425867
H	4.136597	1.712073	2.539884
C	3.834792	-0.660638	3.966302
H	4.682537	-0.014623	4.283097
H	4.248699	-1.423846	3.278549
H	3.461107	-1.171975	4.874238
C	2.206158	1.216569	4.342180
H	3.042841	1.809187	4.769848
H	1.691413	0.711123	5.183868
H	1.487321	1.920712	3.878654
C	0.845813	-2.295312	3.515143
C	1.956003	-3.352654	3.618599
H	1.544794	-4.238325	4.149886
H	2.840495	-3.012851	4.184318
H	2.282009	-3.711361	2.623335
C	0.373084	-1.893092	4.927172
H	-0.046949	-2.781999	5.443619
H	-0.421990	-1.120822	4.892506
H	1.203539	-1.508596	5.553242
C	-0.328156	-2.899906	2.723106
H	0.021012	-3.327177	1.762325
H	-1.101337	-2.145336	2.478798
H	-0.791796	-3.721130	3.309934
C	0.556736	3.308502	1.174440
H	0.535124	2.295291	1.625717
H	0.487290	4.049501	1.997041
H	1.542745	3.433818	0.682646
C	-2.450473	4.021401	0.775247
H	-3.218215	4.284760	0.019643
H	-2.275872	4.921252	1.402434
H	-2.877864	3.233170	1.418815
C	-0.430712	5.075877	-1.117924
H	0.460753	4.975821	-1.764702
H	-0.241464	5.906435	-0.404721
H	-1.287673	5.379865	-1.752607
C	-3.638451	2.434259	-2.349167
H	-4.110797	1.887248	-1.508510
H	-4.216954	2.218356	-3.271756
H	-3.736787	3.519426	-2.139242
C	-1.727204	0.207054	-3.300481
H	-0.683300	-0.060792	-3.549804
H	-2.311927	0.194541	-4.244035
H	-2.144611	-0.580298	-2.647006
C	-1.086483	3.078032	-3.892693
H	-1.111874	4.150009	-3.619739
H	-1.679282	2.951039	-4.823287
H	-0.038895	2.801475	-4.125703
C	-1.870364	1.488787	3.241712
H	-1.064726	0.942707	3.771042
H	-2.478081	2.032557	3.994827
H	-1.388525	2.241073	2.594108
C	-3.515363	-0.953687	3.687508
H	-4.329055	-1.636221	3.377495
H	-3.887233	-0.358887	4.548837
H	-2.672482	-1.575429	4.050599
C	-4.580413	1.121223	1.745020
H	-4.406609	1.737022	0.840760
H	-5.005661	1.774319	2.535462
H	-5.348319	0.362096	1.488837
C	-4.327446	-1.271331	-1.078777
H	-5.214900	-0.974083	-0.483549
H	-4.634226	-2.107144	-1.742572
H	-4.056592	-0.409356	-1.716665
C	-1.576131	-2.702054	-0.925883
H	-1.017453	-2.000745	-1.572825
H	-2.010142	-3.492350	-1.571237
H	-0.844696	-3.175177	-0.240090
C	-3.711383	-3.174212	1.160439
H	-3.048584	-3.529997	1.973097
H	-3.944803	-4.041223	0.506400
H	-4.664797	-2.840350	1.615812
N	1.864284	-1.063084	-1.160755
N	1.693861	-1.178443	1.001639
N	-0.956575	2.016125	-1.011146
N	-2.160850	-0.496653	0.953992
Si	-0.840602	3.516380	-0.102120
Si	-1.811186	1.943224	-2.546985
Si	-2.981703	0.261211	2.314782
Si	-2.920373	-1.818470	0.079671
P	1.166675	-0.633121	2.627899
Co	-0.706530	0.372553	-0.012773

Conformation 26.
Multiplicity: 4
Charge: 0
E(B97-3c) = -4478.408297694679 Hartree
E(M06/def2-TZVP) = -4478.395437685303 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -4476.714917165678 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -4477.087988543492 Hartree
E(PBEh-3c) = -4472.999788385364 Hartree
E(PM6) = -144.64162 Kcal/mol
E(PM7) = -214.11234 Kcal/mol
E(ωB97X-V/def2-TZVP) = -4480.435143783554 Hartree
E(GFN1-xTB) = -139.774534268981 Hartree
E(GFN2-xTB) = -136.962763915174 Hartree
E(GFN-FF) = -18.056701849400 Hartree

Coordinates:

C	0.659939	0.921753	-0.484431
C	1.671749	2.912631	-1.018752
H	1.787752	3.999510	-1.028365
C	2.380919	1.924740	-1.633733
H	3.252862	1.985613	-2.285473
C	-0.371021	3.111034	0.314100
C	-1.574289	3.361716	-0.395822
C	-2.468775	4.293860	0.159472
H	-3.407763	4.516492	-0.365313
C	-2.183986	4.945806	1.366371
H	-2.902860	5.668242	1.781469
C	-0.993662	4.675756	2.046256
H	-0.781650	5.188257	2.995867
C	-0.054356	3.758964	1.533313
C	-1.865434	2.685605	-1.731043

H	-1.474308	1.650641	-1.646385
C	-3.361915	2.580807	-2.040130
H	-3.916905	2.135672	-1.194718
H	-3.518446	1.940507	-2.931086
H	-3.808284	3.570305	-2.271648
C	-1.141429	3.393071	-2.893703
H	-1.499570	4.438659	-2.995996
H	-1.348167	2.869421	-3.849545
H	-0.043490	3.421266	-2.759098
C	1.263682	3.531752	2.265920
H	1.703347	2.593282	1.873138
C	2.255723	4.678891	1.991937
H	2.482302	4.792595	0.914298
H	3.214047	4.498251	2.520511
H	1.845742	5.645180	2.352005
C	1.071547	3.359021	3.781749
H	0.776368	4.312356	4.266350
H	2.021794	3.034839	4.251500
H	0.297625	2.603959	4.014467
C	3.974641	-1.080059	-1.306636
C	4.981389	0.058024	-1.535788
H	4.698699	0.977081	-0.988127
H	5.133050	0.307332	-2.601756
H	5.966806	-0.259620	-1.131003
C	4.516190	-2.375067	-1.943249
H	5.435969	-2.692340	-1.408369
H	4.783591	-2.232684	-3.009375
H	3.791215	-3.210908	-1.878215
C	3.794731	-1.261889	0.214602
H	4.759913	-1.565525	0.673236
H	3.026622	-2.017433	0.460970
H	3.477776	-0.311481	0.688297
C	2.137675	-0.608462	-3.837230
C	3.336993	0.072367	-4.510207
H	3.148103	0.141177	-5.603610
H	4.275511	-0.499620	-4.378120
H	3.503099	1.106322	-4.150658
C	1.969927	-2.030574	-4.419464
H	1.842987	-1.967137	-5.521140
H	1.077046	-2.537176	-4.001525
H	2.849640	-2.673858	-4.221313
C	0.853992	0.191261	-4.128054
H	0.935057	1.249203	-3.810598
H	-0.028906	-0.249010	-3.624697
H	0.658067	0.180733	-5.221385
C	-3.410727	-3.040980	0.061770
H	-2.511904	-3.371627	0.612968
H	-3.614722	-3.765524	-0.753849
H	-4.266116	-3.075985	0.765663
C	-2.030558	-1.239929	-2.106197
H	-2.133611	-0.260217	-2.614991
H	-2.275159	-2.038685	-2.835863
H	-0.956498	-1.367056	-1.839269
C	-4.903267	-0.744120	-1.175956
H	-5.643225	-0.784049	-0.350782
H	-5.241883	-1.458538	-1.956279
H	-4.925677	0.272705	-1.611230
C	-4.362383	-0.992067	2.820916
H	-5.180718	-1.344145	2.159211
H	-4.833557	-0.589041	3.742277
H	-3.758650	-1.876198	3.106543
C	-4.604582	1.694590	1.473162
H	-4.101241	2.614532	1.119797
H	-5.215635	1.963636	2.360700
H	-5.295759	1.345926	0.681356
C	-2.245702	1.194474	3.286409
H	-1.572568	0.482723	3.799896
H	-2.900343	1.658109	4.053396
H	-1.635196	2.001321	2.835525
C	1.071093	0.014134	2.829759
H	2.030884	0.240065	2.323485
H	1.148876	0.337923	3.887607
H	0.285902	0.643950	2.358533
C	2.202759	-2.744792	3.427445
H	2.051933	-3.842520	3.468819
H	2.371641	-2.393930	4.467583
H	3.125486	-2.545629	2.846402
C	-0.771930	-2.249451	3.853488
H	-1.712478	-1.877981	3.404808
H	-0.656805	-1.791619	4.858143
H	-0.876000	-3.344600	3.988135
C	2.178023	-4.536682	0.357716
H	2.770870	-4.073154	-0.453581
H	2.109146	-5.623264	0.138847
H	2.740210	-4.417468	1.303309
C	-0.511203	-5.041723	1.583229
H	0.011548	-5.132908	2.557957
H	-0.532072	-6.052541	1.123827
H	-1.557047	-4.741667	1.790884
C	-0.242624	-4.054234	-1.331682
H	-1.326312	-3.867967	-1.434631
H	-0.044097	-5.101575	-1.641328
H	0.298379	-3.381819	-2.026833
N	0.634111	2.293325	-0.322688
N	1.760575	0.719342	-1.303563
N	-2.403504	-0.236998	0.608933
N	0.331836	-2.171421	1.024942
Si	-3.174586	-1.272942	-0.582418
Si	-3.331697	0.369915	1.971221
Si	0.687086	-1.842832	2.712382
Si	0.407500	-3.825239	0.434195
P	2.170506	-0.911820	-1.933917
Co	-0.497198	-0.532839	0.363749

Conformation 31.
Multiplicity: 4
Charge: 0
E(B97-3c) = -4478.404808017763 Hartree
E(M06/def2-TZVP) = -4478.393357518231 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -4476.711180082665 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -4477.085455220489 Hartree
E(PBEh-3c) = -4473.001523087895 Hartree
E(PM6) = -143.91038 Kcal/mol
E(PM7) = -201.53475 Kcal/mol
E(ωB97X-V/def2-TZVP) = -4480.433794534690 Hartree
E(GFN1-xTB) = -139.769165535525 Hartree
E(GFN2-xTB) = -136.958414179943 Hartree
E(GFN-FF) = -18.057092426330 Hartree

Coordinates:

C	1.067720	-0.395109	0.487151
C	3.246323	-1.113370	0.623948
H	4.118583	-1.707725	0.343223
C	3.056249	-0.215377	1.630519
H	3.754672	0.155352	2.380361
C	1.909209	-2.132725	-1.162617
C	1.147076	-3.318152	-0.975006
C	1.145656	-4.248448	-2.029679
H	0.564302	-5.173853	-1.928505
C	1.860043	-4.017932	-3.211676
H	1.828723	-4.760284	-4.023332
C	2.609208	-2.848792	-3.362735
H	3.172932	-2.678347	-4.291748
C	2.667218	-1.884738	-2.337397
C	0.377966	-3.582905	0.317947
H	-0.196420	-2.654396	0.527737
C	-0.651817	-4.708496	0.189268
H	-1.391139	-4.495589	-0.606375
H	-1.207734	-4.813942	1.141059
H	-0.177191	-5.690731	-0.015707
C	1.315154	-3.871628	1.506899
H	1.894293	-4.802874	1.333839
H	0.718950	-4.012625	2.431852
H	2.038419	-3.056693	1.700446
C	3.592007	-0.678295	-2.497739
H	3.341489	0.051537	-1.700251
C	5.064981	-1.102101	-2.323301
H	5.255151	-1.618202	-1.362229
H	5.734186	-0.219039	-2.374149
H	5.364340	-1.800608	-3.131666
C	3.431235	0.043641	-3.844960
H	3.738201	-0.600461	-4.694170
H	4.074547	0.946149	-3.868939
H	2.389676	0.364779	-4.015566
C	1.920397	2.971747	2.282608
C	3.335450	3.131538	2.850982
H	4.017225	2.318593	2.533279
H	3.346405	3.194411	3.956650
H	3.768746	4.080853	2.467777
C	1.030134	4.124780	2.795256
H	1.469387	5.093394	2.474652
H	0.955049	4.144498	3.899720
H	0.005034	4.067550	2.381222
C	1.964439	3.021692	0.745927
H	2.228011	4.047393	0.412977
H	0.989121	2.752939	0.289490
H	2.726503	2.330205	0.335392
C	1.397582	0.696712	4.406174
C	2.858762	0.382457	4.770060
H	2.911542	0.164748	5.858783
H	3.554335	1.216404	4.569748
H	3.224885	-0.524052	4.252401
C	0.845863	1.763878	5.374787
H	0.802844	1.340055	6.400358
H	-0.181773	2.082500	5.101912
H	1.489707	2.664700	5.416363
C	0.577696	-0.597107	4.563780
H	0.883039	-1.366651	3.825415
H	-0.505672	-0.418133	4.439575
H	0.746535	-1.017439	5.578325
C	-2.111102	-0.809515	2.422420
H	-1.369830	-1.606679	2.631749

H	-2.705946	-0.642684	3.345014
H	-1.547877	0.125978	2.223772
C	-3.826258	-3.104805	1.538098
H	-4.620252	-3.507910	0.881393
H	-4.245136	-3.023863	2.563817
H	-2.999485	-3.840912	1.567423
C	-4.770413	-0.299683	0.866209
H	-4.530353	0.715603	0.496968
H	-5.280636	-0.201959	1.847457
H	-5.497029	-0.746360	0.156422
C	-4.349465	-3.073148	-1.832501
H	-4.023969	-4.017176	-1.350484
H	-4.701800	-3.323420	-2.855922
H	-5.220159	-2.679272	-1.270732
C	-1.684673	-2.709155	-3.125396
H	-0.655243	-2.314248	-3.071846
H	-2.020237	-2.654042	-4.182316
H	-1.641956	-3.782311	-2.848942
C	-3.689242	-0.305215	-2.862896
H	-4.671498	-0.080121	-2.398541
H	-3.855717	-0.470178	-3.947567
H	-3.055985	0.591302	-2.725635
C	-1.460679	3.031093	-3.766247
H	-2.440116	2.543362	-3.944021
H	-0.938021	3.104198	-4.743352
H	-1.651158	4.063384	-3.411155
C	-0.146925	0.336390	-3.426589
H	0.423503	-0.388397	-2.810253
H	0.404907	0.470735	-4.379609
H	-1.119860	-0.121523	-3.678541
C	1.317442	2.851158	-2.528876
H	1.275068	3.847943	-2.046513
H	1.695490	2.989113	-3.563622
H	2.055932	2.235121	-1.978127
C	-3.828118	3.114358	-1.123871
H	-3.747946	3.456981	-2.173658
H	-4.475284	3.833536	-0.578597
H	-4.340414	2.132062	-1.130048
C	-2.491372	2.697932	1.566007
H	-3.162880	1.833175	1.725792
H	-2.999500	3.595128	1.978025
H	-1.568598	2.516684	2.150758
C	-1.334631	4.725801	-0.398184
H	-0.372312	4.775312	0.148849
H	-2.011777	5.491300	0.035662
H	-1.135575	5.015804	-1.449654
N	2.038329	-1.208775	-0.061850
N	1.727444	0.199719	1.558747
N	-2.225937	-1.339812	-0.452613
N	-1.084746	1.768989	-0.974457
Si	-3.215362	-1.385991	0.995248
Si	-2.924608	-1.815910	-1.995048
Si	-0.387872	2.007942	-2.572501
Si	-2.132750	2.996166	-0.272284
P	0.930702	1.373471	2.666975
Co	-0.813575	-0.012358	-0.274470

Conformation 4.
Multiplicity: 4
Charge: 0
E(B97-3c) = -4478.403747200211 Hartree
E(M06/def2-TZVP) = -4478.391927752165 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -4476.710135042079 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -4477.084671617057 Hartree
E(PBEh-3c) = -4473.003533659517 Hartree
E(PM6) = -144.87756 Kcal/mol
E(PM7) = -201.17456 Kcal/mol
E(ωB97X-V/def2-TZVP) = -4480.435918014437 Hartree
E(GFN1-xTB) = -139.765169198715 Hartree
E(GFN2-xTB) = -136.953982957000 Hartree
E(GFN-FF) = -18.060843084280 Hartree

Coordinates:

C	-0.091032	-0.264198	1.148057
C	-0.034918	-1.169120	3.257753
H	0.230557	-1.901072	4.024065
C	-0.747401	-0.009131	3.337379
H	-1.217726	0.466616	4.197902
C	1.264391	-2.366098	1.528146
C	0.733551	-3.582349	1.030197
C	1.652091	-4.569517	0.624830
H	1.276779	-5.516378	0.212402
C	3.032256	-4.365658	0.740842
H	3.731720	-5.143885	0.399913
C	3.524846	-3.191057	1.321256
H	4.608710	-3.064483	1.455504
C	2.653331	-2.172308	1.749800
C	-0.766537	-3.857896	1.036795
H	-1.279662	-2.898448	0.822187
C	-1.228172	-4.884256	-0.006217
H	-0.882620	-4.629943	-1.024840
H	-2.335063	-4.928202	-0.021840
H	-0.867236	-5.904850	0.237863
C	-1.213017	-4.331113	2.436712
H	-0.702958	-5.279745	2.703623
H	-2.306745	-4.514833	2.450107
H	-0.988806	-3.592210	3.228306
C	3.184695	-0.984874	2.549624
H	2.455990	-0.154183	2.443661
C	3.269252	-1.360367	4.044816
H	2.303028	-1.706834	4.455955
H	3.600558	-0.488066	4.644808
H	4.005699	-2.176681	4.194366
C	4.552466	-0.465540	2.090593
H	5.358534	-1.201935	2.287708
H	4.811148	0.454882	2.651479
H	4.564853	-0.224403	1.015695
C	-0.333169	3.284749	2.793280
C	1.111954	2.759659	2.741049
H	1.458962	2.593330	1.703382
H	1.229057	1.808709	3.298236
H	1.790415	3.506941	3.204442
C	-0.778296	3.411676	4.256619
H	-0.082979	4.097691	4.787623
H	-0.744475	2.444956	4.795358
H	-1.795136	3.836567	4.360029
C	-0.372781	4.674339	2.117817
H	0.292743	5.372488	2.668894
H	-1.388175	5.116276	2.114622
H	-0.020644	4.624204	1.067799
C	-3.185878	2.121910	2.168546
C	-3.531573	1.531754	3.544255
H	-4.624473	1.646881	3.710623
H	-3.019649	2.036768	4.383799
H	-3.318348	0.446914	3.592100
C	-3.709610	3.569216	2.079044
H	-4.816910	3.558292	2.163740
H	-3.461983	4.045176	1.108887
H	-3.322437	4.211263	2.894326
C	-3.872172	1.268282	1.088593
H	-3.525189	0.217882	1.121144
H	-3.666206	1.651064	0.073612
H	-4.971288	1.266897	1.251248
C	0.763767	-0.655053	-4.677539
H	-0.167119	-0.120796	-4.414111
H	0.537465	-1.377209	-5.489178
H	1.485746	0.090996	-5.068614
C	0.343786	-2.888218	-2.529503
H	0.899339	-3.474039	-1.770896
H	0.031483	-3.571680	-3.345755
H	-0.571661	-2.494630	-2.047400
C	3.061814	-2.387107	-3.703460
H	3.799440	-1.703840	-4.170203
H	2.776895	-3.139187	-4.469795
H	3.559897	-2.921706	-2.870073
C	3.586402	1.573051	-3.277877
H	3.718836	0.903786	-4.153134
H	4.536737	2.131120	-3.139182
H	2.796284	2.306868	-3.533289
C	4.694724	-0.567107	-1.462920
H	4.462222	-1.429233	-0.806883
H	5.536773	0.000941	-1.014466
H	5.049703	-0.969955	-2.430763
C	3.073040	1.760280	-0.246260
H	2.388015	2.600912	-0.468206
H	4.066443	2.184533	0.005967
H	2.686175	1.228880	0.644176
C	-2.773890	3.463155	-1.777983
H	-3.817363	3.114973	-1.900279
H	-2.682106	4.446937	-2.285050
H	-2.577832	3.620540	-0.699268
C	-1.700233	2.329473	-4.383290
H	-0.916951	1.748962	-4.909650
H	-1.642927	3.380806	-4.735683
H	-2.686195	1.927591	-4.694758
C	0.191595	3.054327	-2.076473
H	0.316060	3.114628	-0.975573
H	0.252533	4.085286	-2.482645
H	1.027338	2.462983	-2.493537
C	-2.657585	-1.321526	-3.948190
H	-2.604089	-0.594134	-4.782971
H	-3.538264	-1.974907	-4.126018
H	-1.750560	-1.952102	-3.993018
C	-3.097479	-1.802199	-0.973341
H	-2.350235	-2.607896	-1.100224
H	-4.099736	-2.265705	-1.084237
H	-3.007439	-1.413734	0.060113
C	-4.537385	0.458780	-2.452839
H	-4.879219	0.951623	-1.522566
H	-5.304686	-0.290681	-2.740134
H	-4.510198	1.223976	-3.254857
N	0.362340	-1.311280	1.931656

N	-0.777679	0.535043	2.054178
N	1.682324	-0.344506	-1.829911
N	-1.535731	0.633796	-1.839492
Si	1.474917	-1.499304	-3.139695
Si	3.176185	0.563474	-1.714077
Si	-1.475584	2.267075	-2.494906
Si	-2.861003	-0.436287	-2.276212
P	-1.355424	2.176735	1.593128
Co	0.045973	0.046738	-0.871347

Conformation 7.
Multiplicity: 4
Charge: 0
E(B97-3c) = -4478.403849343878 Hartree
E(M06/def2-TZVP) = -4478.392241751249 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -4476.710100065953 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -4477.084187301767 Hartree
E(PBEh-3c) = -4473.001684774375 Hartree
E(PM6) = -143.67055 Kcal/mol
E(PM7) = -196.38174 Kcal/mol
E(ωB97X-V/def2-TZVP) = -4480.432182199037 Hartree
E(GFN1-xTB) = -139.766908000021 Hartree
E(GFN2-xTB) = -136.956592775997 Hartree
E(GFN-FF) = -18.064664554368 Hartree

Coordinates:

C	-1.177992	-0.050136	-0.283416
C	-3.462870	-0.265390	-0.381536
H	-4.445241	-0.631592	-0.074660
C	-3.088648	0.522230	-1.429373
H	-3.693089	0.995780	-2.204446
C	-2.336702	-1.429499	1.487919
C	-1.780314	-2.736360	1.435398
C	-1.800976	-3.488224	2.624954
H	-1.364638	-4.495086	2.633569
C	-2.377934	-2.986954	3.798550
H	-2.367801	-3.593751	4.716472
C	-3.000135	-1.736578	3.792943
H	-3.499136	-1.372044	4.702851
C	-3.009571	-0.933141	2.636055
C	-1.238137	-3.336606	0.136700
H	-0.448015	-2.646112	-0.234156
C	-0.609743	-4.724096	0.312872
H	0.211349	-4.730709	1.053434
H	-0.190336	-5.065557	-0.652986
H	-1.368525	-5.471560	0.625271
C	-2.315196	-3.434742	-0.964555
H	-3.144915	-4.096519	-0.639846
H	-1.870026	-3.875185	-1.879677
H	-2.748114	-2.458255	-1.247336
C	-3.852320	0.342697	2.627544
H	-3.578628	0.936031	1.731645
C	-5.344353	-0.036878	2.513001
H	-5.549106	-0.716631	1.661777
H	-5.973599	0.868733	2.392657
H	-5.680003	-0.564191	3.429597
C	-3.649198	1.255718	3.844253
H	-3.922939	0.751497	4.793448
H	-4.297051	2.150794	3.751574
H	-2.604154	1.596035	3.928694
C	-1.562987	3.294863	-2.542264
C	-1.966430	3.668018	-1.104673
H	-1.124938	3.556821	-0.393021
H	-2.807129	3.052943	-0.727915
H	-2.287057	4.731228	-1.079856
C	-2.772846	3.431739	-3.476364
H	-3.153360	4.475060	-3.424068
H	-3.615923	2.772359	-3.193143
H	-2.516065	3.233187	-4.534407
C	-0.454230	4.268428	-3.005319
H	-0.857596	5.303147	-3.031129
H	-0.078996	4.031192	-4.020293
H	0.411079	4.255845	-2.312911
C	-0.855195	0.623879	-4.071386
C	-2.274063	0.246950	-4.521905
H	-2.205034	-0.315607	-5.478180
H	-2.922704	1.122654	-4.703895
H	-2.773069	-0.422469	-3.794803
C	-0.146573	1.424685	-5.180041
H	-0.064001	0.790826	-6.088435
H	0.880391	1.720859	-4.889278
H	-0.707497	2.336668	-5.466024
C	-0.070354	-0.668950	-3.785673
H	-0.592714	-1.292405	-3.032663
H	0.940127	-0.456731	-3.388023
H	0.025942	-1.269492	-4.715290
C	4.029183	-0.548405	2.421841
H	4.131867	-0.372372	1.335553
H	4.799036	-1.284638	2.732803
H	4.232273	0.409443	2.943000
C	1.965744	-2.848547	2.037087
H	1.036462	-3.268773	2.470141
H	2.798207	-3.551919	2.244332
H	1.833582	-2.789900	0.940456
C	2.186025	-1.440157	4.675052
H	2.454268	-0.545732	5.272061
H	2.919320	-2.236427	4.924805
H	1.183427	-1.787595	4.995405
C	2.037467	2.436696	3.764383
H	2.731170	1.846925	4.398580
H	1.656717	3.278162	4.381310
H	2.626980	2.866807	2.930566
C	-0.280867	0.790365	4.761249
H	-0.980770	-0.047683	4.576807
H	-0.846027	1.631837	5.213401
H	0.459707	0.454318	5.511225
C	-0.593802	2.483240	2.195599
H	-0.045334	3.011114	1.391837
H	-1.034055	3.252806	2.862934
H	-1.418315	1.911555	1.726640
C	2.349056	2.629412	-0.086797
H	1.274968	2.772519	-0.323727
H	2.857618	3.608553	-0.207501
H	2.432013	2.316034	0.970546
C	2.985356	2.055083	-2.994513
H	3.278111	1.335863	-3.782942
H	3.650153	2.940899	-3.076777
H	1.949478	2.390244	-3.192457
C	4.979908	1.278923	-0.862202
H	5.191488	0.927783	0.166740
H	5.401388	2.301087	-0.966385
H	5.530391	0.622183	-1.566406
C	4.481258	-2.350660	-0.662656
H	5.282110	-1.593506	-0.549582
H	4.918227	-3.227147	-1.187094
H	4.182063	-2.675815	0.351558
C	1.789506	-3.102275	-1.875115
H	1.546009	-3.566341	-0.901246
H	2.256744	-3.889305	-2.503286
H	0.842961	-2.797067	-2.359938
C	3.760410	-1.357792	-3.414669
H	3.004303	-1.017004	-4.150192
H	4.190998	-2.309889	-3.790122
H	4.577834	-0.609352	-3.395426
N	-2.298767	-0.604301	0.306542
N	-1.702398	0.649047	-1.361261
N	1.091379	0.001874	2.161547
N	2.290445	-0.211113	-0.992314
Si	2.271249	-1.141618	2.797070
Si	0.588662	1.353794	3.160746
Si	3.112725	1.332708	-1.235422
Si	3.021268	-1.665689	-1.676208
P	-0.638560	1.611033	-2.439333
Co	0.798664	-0.118704	0.253529

Conformation 9.
Multiplicity: 4
Charge: 0
E(B97-3c) = -4478.408218852044 Hartree
E(M06/def2-TZVP) = -4478.397373388160 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -4476.714735189170 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -4477.088699543199 Hartree
E(PBEh-3c) = -4473.006023753136 Hartree
E(PM6) = -146.48849 Kcal/mol
E(PM7) = -214.72955 Kcal/mol
E(ωB97X-V/def2-TZVP) = -4480.436636196658 Hartree
E(GFN1-xTB) = -139.772890041799 Hartree
E(GFN2-xTB) = -136.962622835129 Hartree
E(GFN-FF) = -18.065813191970 Hartree

Coordinates:

C	0.590487	0.170859	-1.041947
C	1.632658	-0.256072	-3.040777
H	1.721547	-0.648984	-4.056752
C	2.502234	0.468866	-2.279578
H	3.516464	0.805874	-2.497410
C	-0.723471	-0.977680	-2.880672
C	-0.712957	-2.324019	-3.328865
C	-1.866834	-2.809224	-3.976906
H	-1.884970	-3.852392	-4.324622
C	-2.984118	-1.996804	-4.172479
H	-3.880375	-2.398428	-4.668649
C	-2.961312	-0.664823	-3.741228
H	-3.838813	-0.029657	-3.918931
C	-1.834657	-0.116461	-3.103072
C	0.477707	-3.262780	-3.164002
H	1.191906	-2.790214	-2.461803
C	0.063975	-4.615798	-2.557358
H	-0.544089	-4.483412	-1.642954
H	0.963343	-5.207311	-2.292895
H	-0.527662	-5.220202	-3.275195

C	1.200347	-3.487306	-4.506157
H	0.527314	-3.975723	-5.240809
H	2.082739	-4.144840	-4.367401
H	1.550998	-2.541195	-4.965097
C	-1.792747	1.366777	-2.746923
H	-1.365222	1.437274	-1.724614
C	-0.879831	2.135203	-3.723567
H	0.163024	1.763752	-3.717076
H	-0.855340	3.212442	-3.461628
H	-1.263020	2.049321	-4.761618
C	-3.174759	2.023120	-2.706773
H	-3.628888	2.097680	-3.716746
H	-3.092151	3.054985	-2.311506
H	-3.868566	1.466165	-2.050075
C	2.568156	3.516804	-0.715273
C	3.305130	3.520221	-2.062219
H	2.744846	2.959002	-2.834405
H	4.331914	3.115700	-2.003420
H	3.384927	4.568678	-2.423105
C	3.256028	4.480193	0.271401
H	3.164737	5.519679	-0.109034
H	4.336079	4.264678	0.389420
H	2.781485	4.452063	1.274528
C	1.123619	3.996974	-0.949531
H	1.137339	4.968140	-1.489452
H	0.576118	4.140451	0.000556
H	0.547364	3.279059	-1.565530
C	4.085944	1.156451	0.704138
C	5.281295	1.432736	-0.217223
H	6.180820	0.933430	0.203790
H	5.516903	2.511565	-0.299271
H	5.140867	1.025677	-1.237535
C	4.376987	1.742292	2.103716
H	5.292550	1.267729	2.516660
H	3.547754	1.541562	2.808893
H	4.552007	2.834984	2.079389
C	3.861641	-0.359696	0.842753
H	3.803803	-0.859658	-0.144348
H	2.922136	-0.578932	1.391673
H	4.710352	-0.809245	1.400453
C	-4.127534	-1.819949	2.307480
H	-3.317875	-1.927422	3.057609
H	-4.665239	-2.788624	2.237181
H	-4.844543	-1.067227	2.695684
C	-2.507048	-2.765748	-0.136671
H	-2.147305	-2.522124	-1.154497
H	-3.205931	-3.623617	-0.225841
H	-1.647862	-3.104066	0.469611
C	-4.925541	-1.046148	-0.540224
H	-5.641480	-0.284448	-0.178349
H	-5.472356	-2.008437	-0.632768
H	-4.588640	-0.755872	-1.555466
C	-1.817830	3.017516	0.805658
H	-0.763414	2.683062	0.877274
H	-1.924448	3.936052	1.418685
H	-2.005432	3.286496	-0.253246
C	-3.190793	1.725708	3.260785
H	-3.876339	0.930044	3.616224
H	-3.634407	2.703235	3.546235
H	-2.237878	1.612943	3.807645
C	-4.743607	2.130315	0.757503
H	-4.858758	2.085547	-0.341862
H	-4.939856	3.175828	1.077592
H	-5.529181	1.495148	1.214856
C	0.482338	1.910703	3.513217
H	1.387348	2.282732	2.994132
H	0.429002	2.386751	4.514680
H	-0.391297	2.254577	2.931528
C	2.167736	-0.267753	4.728186
H	2.173243	-1.255416	5.229019
H	2.240908	0.505779	5.521934
H	3.083556	-0.202853	4.107538
C	-0.853601	-0.559412	4.838348
H	-1.806473	-0.601181	4.275961
H	-0.994777	0.107695	5.714228
H	-0.644973	-1.579036	5.222399
C	-0.482945	-3.603614	2.862103
H	-0.415650	-3.571960	3.968959
H	-0.386376	-4.665436	2.552070
H	-1.495052	-3.252374	2.585207
C	1.152426	-2.992246	0.280818
H	0.308741	-2.651898	-0.346967
H	1.252732	-4.088635	0.151503
H	2.072696	-2.510332	-0.105775
C	2.480011	-3.100730	2.995816
H	3.368310	-2.490433	2.742343
H	2.689180	-4.148342	2.690730
H	2.363926	-3.094713	4.096923
N	0.468846	-0.418252	-2.287742
N	1.848892	0.752190	-1.080079
N	-2.393104	0.117400	0.752811
N	0.554342	-0.810111	2.175115
Si	-3.434043	-1.295206	0.615864
Si	-3.006102	1.646299	1.370026
Si	0.571162	0.027299	3.723224
Si	0.895470	-2.533468	2.101775
P	2.363446	1.861000	0.240825
Co	-0.472380	-0.096766	0.681245

AQINUK

Conformation 13.
Multiplicity: 2
Charge: 0
E(B97-3c) = -14780.095388065132 Hartree
E(M06/def2-TZVP) = -14775.725164253348 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -14773.096709391895 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -14773.633988185265 Hartree
E(PBEh-3c) = -14765.504047416023 Hartree
E(PM6) = 117.70812 Kcal/mol
E(PM7) = 60.57875 Kcal/mol
E(ωB97X-V/def2-TZVP) = -14776.333673339606 Hartree
E(GFN1-xTB) = -208.694566201214 Hartree
E(GFN2-xTB) = -205.331427868363 Hartree
E(GFN-FF) = -24.580282218097 Hartree

Coordinates:

C	1.788253	2.709541	0.888428
C	2.277646	3.934097	0.273004
C	1.622811	4.064619	-0.940796
C	0.732941	2.920224	-1.067260
C	-0.247300	2.710609	-2.067635
C	-0.844599	1.449927	-2.291035
C	-1.945794	1.216881	-3.204714
H	-2.494404	1.997843	-3.740570
C	-2.155122	-0.139544	-3.237092
H	-2.909266	-0.693048	-3.805452
C	-1.180980	-0.735799	-2.344472
C	-0.988998	-2.126448	-2.187769
C	-0.113131	-2.666604	-1.214507
C	0.407085	-4.024634	-1.162970
C	1.074650	-4.154925	0.044013
C	0.959318	-2.877249	0.731529
C	1.342092	-2.588981	2.064515
C	1.483331	-1.267318	2.542620
C	1.742859	-0.920517	3.925819
H	1.757932	-1.628497	4.760546
C	1.943208	0.437215	3.963937
H	2.156022	1.063914	4.835787
C	1.805828	0.919879	2.603944
C	2.057041	2.250282	2.200677
C	-0.720775	3.859700	-2.880007
C	-0.645622	3.854177	-4.286880
H	-0.201472	2.985684	-4.795545
C	-1.086719	4.945127	-5.048801
H	-0.991628	4.910371	-6.141946
C	-1.635212	6.073141	-4.402161
C	-1.735322	6.083028	-2.992570
H	-2.175275	6.966052	-2.507200
C	-1.279102	4.997206	-2.249001
H	-1.352931	5.017026	-1.151281
C	-2.005232	7.246833	-6.464002
H	-2.599564	6.420090	-6.917385
H	-0.944814	7.112609	-6.784198
C	-2.531138	8.602280	-6.909941
H	-3.585018	8.702111	-6.569065
H	-2.561601	8.606586	-8.021516
C	-1.704042	9.786295	-6.399432
H	-1.650037	9.727342	-5.291989
H	-0.656665	9.679036	-6.760570
C	-2.264820	11.141870	-6.827746
H	-1.647461	11.978996	-6.444694
H	-3.297779	11.288578	-6.448442
H	-2.304527	11.234793	-7.933556
C	-1.784051	-3.044568	-3.041074
C	-1.722467	-2.993738	-4.454059
H	-1.050282	-2.268227	-4.935585
C	-2.465383	-3.874492	-5.238744
H	-2.404474	-3.855652	-6.336456
C	-3.311582	-4.830399	-4.632635
C	-3.401471	-4.880148	-3.225130
H	-4.060176	-5.602279	-2.725398
C	-2.638208	-3.997663	-2.450596
H	-2.705625	-4.046324	-1.353242
C	-4.832008	-6.659595	-4.930110
H	-5.640427	-6.197070	-4.314668
H	-4.237985	-7.316166	-4.253833
C	-5.429747	-7.450861	-6.084844
H	-4.598873	-7.898667	-6.672325
H	-5.939634	-6.734053	-6.762265
C	-6.412299	-8.542511	-5.640642

H	-6.884733	-8.973777	-6.548379
H	-7.244040	-8.076672	-5.065933
C	-5.785292	-9.670279	-4.815464
H	-6.527599	-10.460580	-4.584949
H	-5.383238	-9.309640	-3.846412
H	-4.946548	-10.149656	-5.362621
C	1.550123	-3.707625	3.016310
C	0.522843	-4.647135	3.240148
H	-0.435481	-4.525435	2.713091
C	0.696436	-5.732704	4.105672
H	-0.129950	-6.442127	4.245184
C	1.929229	-5.907470	4.771584
C	2.959531	-4.961252	4.572880
H	3.913289	-5.115172	5.097893
C	2.767929	-3.878197	3.715802
H	3.588026	-3.164620	3.547509
C	1.303940	-8.021712	5.733139
H	0.268472	-7.645161	5.888993
H	1.599142	-8.545868	6.664956
C	1.390104	-8.976920	4.541827
H	1.222764	-8.408829	3.600893
H	2.430697	-9.360204	4.490009
C	0.397006	-10.144864	4.620639
H	0.523491	-10.673622	5.592200
H	0.667915	-10.887935	3.841262
C	-1.068828	-9.738664	4.438483
H	-1.738658	-10.621692	4.455080
H	-1.221349	-9.222009	3.467687
H	-1.418148	-9.052082	5.237011
C	2.569829	3.202994	3.217204
C	1.843407	4.370183	3.526764
H	0.894065	4.563086	3.004540
C	2.300530	5.288498	4.480484
H	1.701597	6.183038	4.694960
C	3.522555	5.053266	5.145632
C	4.258438	3.883427	4.850646
H	5.210514	3.719712	5.375915
C	3.783048	2.972727	3.908423
H	4.373479	2.075339	3.671340
C	3.392108	7.098329	6.396209
H	2.380578	6.864268	6.802238
H	3.246943	7.706342	5.471727
C	4.208280	7.873348	7.421704
H	3.545053	8.673871	7.813944
H	4.420827	7.199859	8.280955
C	5.509337	8.508465	6.907842
H	5.877920	9.209814	7.687544
H	5.270723	9.145007	6.025955
C	6.627767	7.526803	6.548119
H	7.550933	8.066830	6.255172
H	6.338560	6.860427	5.713154
H	6.879004	6.875307	7.410985
N	0.920411	2.085224	0.015529
N	-0.426936	0.253099	-1.745541
N	0.309272	-1.981977	-0.093398
N	1.479706	-0.126813	1.765696
O	-2.091068	7.181429	-5.041652
O	-3.992164	-5.647487	-5.477737
O	2.216661	-6.929401	5.622331
O	4.066763	5.882514	6.074328
Cu	0.563389	0.059091	-0.010550
Br	3.682255	5.044376	0.835616
Br	2.031334	5.374041	-2.221258
Br	0.419119	-5.322204	-2.518822
Br	2.108715	-5.648911	0.518500

Conformation 15.
Multiplicity: 2
Charge: 0
E(B97-3c) = -14780.094958319898 Hartree
E(M06/def2-TZVP) = -14775.724403138262 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -14773.096372453192 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -14773.633503454097 Hartree
E(PBEh-3c) = -14765.504187436916 Hartree
E(PM6) = 120.01410 Kcal/mol
E(PM7) = 62.93994 Kcal/mol
E(ωB97X-V/def2-TZVP) = -14776.333607107197 Hartree
E(GFN1-xTB) = -208.695170886094 Hartree
E(GFN2-xTB) = -205.329612273747 Hartree
E(GFN-FF) = -24.581360634561 Hartree

Coordinates:

C	-0.878497	2.754524	0.715242
C	-1.939705	3.407405	1.466949
C	-2.644332	2.409031	2.119449
C	-2.010044	1.146430	1.771374
C	-2.279482	-0.125497	2.331870
C	-1.832803	-1.326374	1.736663
C	-1.954004	-2.635709	2.347012
H	-2.312196	-2.825079	3.363869
C	-1.522074	-3.549071	1.417438
H	-1.455682	-4.636765	1.520662
C	-1.140913	-2.798293	0.237383
C	-0.760670	-3.381882	-0.991565
C	-0.286968	-2.613194	-2.082905
C	-0.179748	-3.038174	-3.470715
C	0.483283	-2.030154	-4.151304
C	0.785608	-0.990631	-3.178668
C	1.594003	0.154343	-3.378694
C	1.592894	1.249322	-2.485875
C	2.508140	2.370557	-2.567590
H	3.350448	2.446988	-3.262552
C	2.116662	3.273617	-1.610522
H	2.573173	4.237548	-1.364633
C	0.958645	2.706777	-0.947908
C	0.179195	3.384761	0.015122
C	-3.001889	-0.217233	3.625946
C	-4.195431	-0.954143	3.757174
H	-4.614434	-1.455936	2.872331
C	-4.880030	-1.029290	4.978341
H	-5.818485	-1.596201	5.034219
C	-4.360803	-0.368983	6.112210
C	-3.152523	0.355237	5.999481
H	-2.757933	0.854070	6.896321
C	-2.492381	0.432831	4.775505
H	-1.557435	1.007316	4.694270
C	-6.178485	-1.061417	7.520647
H	-6.046609	-2.144945	7.295061
H	-6.939339	-0.660200	6.809955
C	-6.628979	-0.857192	8.958870
H	-5.845695	-1.264136	9.635366
H	-7.536221	-1.478896	9.122944
C	-6.917851	0.604174	9.315797
H	-6.012760	1.207302	9.092321
H	-7.714817	0.991214	8.642065
C	-7.331192	0.797651	10.774389
H	-7.532212	1.863262	11.004005
H	-6.536039	0.451421	11.467353
H	-8.250951	0.224566	11.016690
C	-0.817381	-4.860410	-1.111964
C	0.344835	-5.590484	-1.432252
H	1.288958	-5.047640	-1.590371
C	0.326281	-6.985684	-1.554151
H	1.255664	-7.515442	-1.799951
C	-0.883563	-7.686206	-1.363011
C	-2.055916	-6.968271	-1.035260
H	-2.990673	-7.531157	-0.899157
C	-2.017987	-5.580847	-0.905750
H	-2.940745	-5.029497	-0.672273
C	0.118147	-9.818221	-1.826418
H	0.935456	-9.662915	-1.082320
H	0.502021	-9.481161	-2.817184
C	-0.276782	-11.287686	-1.882180
H	0.555852	-11.819357	-2.390676
H	-1.160613	-11.387506	-2.549875
C	-0.550904	-11.964049	-0.530267
H	0.332836	-11.811595	0.129772
H	-0.606515	-13.060964	-0.701445
C	-1.820053	-11.505044	0.192936
H	-1.975806	-12.082826	1.126539
H	-2.716599	-11.649959	-0.445281
H	-1.778633	-10.430407	0.454372
C	2.526363	0.202181	-4.533213
C	3.513611	-0.790462	-4.696116
H	3.581468	-1.603117	-3.957055
C	4.410786	-0.765009	-5.770862
H	5.169152	-1.554503	-5.853379
C	4.324923	0.266716	-6.730312
C	3.344055	1.271948	-6.574796
H	3.288183	2.064291	-7.335178
C	2.467738	1.241892	-5.490627
H	1.696852	2.020253	-5.390536
C	6.193431	-0.537951	-8.033030
H	6.428962	-0.451486	-9.112574
H	5.857407	-1.583833	-7.855793
C	7.424633	-0.202758	-7.188751
H	7.214688	-0.417559	-6.119826
H	8.231245	-0.907043	-7.492650
C	7.910489	1.247625	-7.324453
H	8.776460	1.387301	-6.642939
H	7.115685	1.926847	-6.948711
C	8.302540	1.658995	-8.744895
H	8.721323	2.685146	-8.763183
H	7.431395	1.653193	-9.431576
H	9.070795	0.978614	-9.170014
C	0.526358	4.792001	0.335550
C	0.863906	5.152888	1.655457
H	0.865025	4.377739	2.436607
C	1.196554	6.470383	1.994710
H	1.458991	6.707648	3.033748
C	1.185090	7.470646	0.999447
C	0.854759	7.122473	-0.329872

H	0.846526	7.916880	-1.090120
C	0.539463	5.803808	-0.653877
H	0.263187	5.546844	-1.687145
C	1.789386	9.205812	2.544549
H	2.699040	8.667516	2.898807
H	0.954492	8.939645	3.235479
C	2.027032	10.709797	2.549500
H	2.496442	10.952765	3.526801
H	2.787931	10.946443	1.773598
C	0.781589	11.589420	2.360063
H	1.064339	12.637758	2.598089
H	0.025259	11.305019	3.126142
C	0.146994	11.545308	0.967349
H	-0.701217	12.255936	0.894973
H	-0.227706	10.534297	0.717841
H	0.884242	11.821098	0.184731
N	-1.002256	1.387978	0.859287
N	-1.293314	-1.446796	0.472289
N	0.234386	-1.341405	-1.962308
N	0.688195	1.455784	-1.464906
O	-4.941380	-0.374412	7.340125
O	-1.019666	-9.034129	-1.469106
O	5.113412	0.376637	-7.833281
O	1.473918	8.780124	1.219050
Cu	-0.335792	0.011865	-0.518641
Br	-2.460607	5.209874	1.425872
Br	-4.237666	2.693479	3.068911
Br	-0.964392	-4.527780	-4.300325
Br	0.704978	-1.988249	-6.014120

Conformation 17.
Multiplicity: 2
Charge: 0
E(B97-3c) = -14780.097572059831 Hartree
E(M06/def2-TZVP) = -14775.727575084500 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -14773.098535778976 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -14773.635880265881 Hartree
E(PBEh-3c) = -14765.507170753935 Hartree
E(PM6) = 117.13815 Kcal/mol
E(PM7) = 59.28318 Kcal/mol
E(ωB97X-V/def2-TZVP) = -14776.335895198592 Hartree
E(GFN1-xTB) = -208.697099422761 Hartree
E(GFN2-xTB) = -205.332557611256 Hartree
E(GFN-FF) = -24.583520275293 Hartree

Coordinates:

C	-1.029405	0.768935	2.972256
C	-0.669987	0.742495	4.382054
C	0.705755	0.591574	4.444354
C	1.186573	0.520605	3.072703
C	2.536642	0.513926	2.643388
C	2.914560	0.113798	1.342244
C	4.263475	0.199189	0.817368
H	5.107575	0.674898	1.326467
C	4.250294	-0.408757	-0.413569
H	5.081181	-0.531923	-1.115632
C	2.892528	-0.860892	-0.643144
C	2.487242	-1.630296	-1.755845
C	1.128789	-1.931692	-2.019060
C	0.616554	-2.937293	-2.938431
C	-0.753597	-2.748401	-3.018678
C	-1.079227	-1.630857	-2.145393
C	-2.333254	-0.984418	-2.020528
C	-2.642682	-0.138567	-0.932190
C	-3.860277	0.639950	-0.820037
H	-4.616461	0.741696	-1.604769
C	-3.852559	1.211921	0.428057
H	-4.602062	1.875597	0.870621
C	-2.628635	0.785965	1.077563
C	-2.298110	1.072045	2.421507
C	3.596309	0.997093	3.563602
C	4.701389	0.195998	3.913550
H	4.768687	-0.827063	3.514692
C	5.693866	0.658094	4.789043
H	6.528568	-0.004638	5.052244
C	5.601343	1.959619	5.326641
C	4.507457	2.780157	4.969909
H	4.457464	3.794635	5.390866
C	3.522590	2.301376	4.109425
H	2.670248	2.944539	3.843521
C	7.629240	1.729320	6.591365
H	8.239925	1.448930	5.702128
H	7.280078	0.784101	7.070524
C	8.445810	2.556773	7.571720
H	8.768443	3.491041	7.062066
H	9.374972	1.991062	7.802574
C	7.700854	2.899681	8.865593
H	6.757658	3.422936	8.601904
H	7.393721	1.955138	9.367953
C	8.526718	3.754459	9.826325
H	7.963838	3.989343	10.751863
H	8.817677	4.718483	9.359053
H	9.463215	3.238755	10.126235
C	3.526806	-2.086917	-2.710965
C	4.604860	-2.907094	-2.304356
H	4.678558	-3.212232	-1.250022
C	5.537608	-3.377822	-3.228233
H	6.359110	-4.043247	-2.925832
C	5.431429	-3.027154	-4.592532
C	4.388346	-2.170646	-5.004886
H	4.293425	-1.859622	-6.053683
C	3.450988	-1.718410	-4.069871
H	2.627708	-1.067836	-4.401412
C	6.189125	-3.495589	-6.833249
H	7.169608	-3.801787	-7.248484
H	6.007900	-2.449453	-7.168483
C	5.080481	-4.430382	-7.323805
H	5.122149	-4.427582	-8.435990
H	4.087709	-4.015366	-7.050997
C	5.181366	-5.867487	-6.792208
H	4.334804	-6.449984	-7.214124
H	5.018845	-5.854680	-5.692993
C	6.501610	-6.574386	-7.104172
H	6.476510	-7.632823	-6.775896
H	7.356245	-6.093710	-6.585789
H	6.720971	-6.569370	-8.193173
C	-3.348071	-1.147213	-3.091461
C	-3.035380	-0.799436	-4.427605
H	-2.031786	-0.411587	-4.658222
C	-3.974193	-0.937456	-5.447154
H	-3.737979	-0.662681	-6.485227
C	-5.262765	-1.444249	-5.164778
C	-5.593940	-1.791800	-3.837786
H	-6.585247	-2.192486	-3.588819
C	-4.642396	-1.633670	-2.820640
H	-4.899746	-1.925044	-1.791537
C	-7.416750	-2.079110	-6.014883
H	-7.978288	-1.426690	-5.306959
H	-7.350247	-3.090436	-5.550629
C	-8.123274	-2.141054	-7.362222
H	-9.155245	-2.513175	-7.178767
H	-8.226253	-1.105901	-7.751340
C	-7.423234	-3.017790	-8.410952
H	-6.409982	-2.602822	-8.596027
H	-7.975315	-2.921343	-9.370013
C	-7.312884	-4.495478	-8.029765
H	-6.856973	-5.088380	-8.847771
H	-8.309155	-4.936352	-7.813611
H	-6.679964	-4.645837	-7.130975
C	-3.310387	1.771733	3.251495
C	-3.011539	3.015876	3.843014
H	-2.015298	3.456482	3.686723
C	-3.951535	3.706400	4.617543
H	-3.676769	4.676652	5.051374
C	-5.230276	3.147121	4.830580
C	-5.543478	1.901636	4.241111
H	-6.541027	1.477282	4.425101
C	-4.601460	1.232436	3.460949
H	-4.851018	0.255288	3.021769
C	-6.027917	5.007289	6.147671
H	-5.030454	5.080131	6.635593
H	-6.792521	5.072781	6.948710
C	-6.236156	6.129975	5.131885
H	-6.062308	7.096494	5.655397
H	-5.457412	6.067394	4.341110
C	-7.624795	6.122107	4.485235
H	-8.397315	6.219141	5.280535
H	-7.795478	5.127451	4.021291
C	-7.807985	7.224291	3.442397
H	-8.818870	7.194156	2.988636
H	-7.069583	7.125228	2.619494
H	-7.671190	8.232222	3.887576
N	0.104961	0.549367	2.216640
N	2.089404	-0.492314	0.416583
N	0.067951	-1.218264	-1.499278
N	-1.887791	0.004856	0.214591
O	6.504792	2.505514	6.181320
O	6.380771	-3.546533	-5.416954
O	-6.105985	-1.557380	-6.223619
O	-6.213856	3.705674	5.586555
Cu	0.094572	-0.281471	0.333179
Br	-1.805650	0.682185	5.875081
Br	1.662994	0.310826	6.033731
Br	1.525476	-4.386552	-3.713764
Br	-1.924943	-3.901236	-3.925051

Conformation 20.
Multiplicity: 2
Charge: 0
E(B97-3c) = -14780.091353752483 Hartree
E(M06/def2-TZVP) = -14775.721276112887 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -14773.092961385832 Hartree

E(PBE0 - D3(BJ)/def2-TZVP) = -14773.629674476910 Hartree
E(PBEh-3c) = -14765.499354599709 Hartree
E(PM6) = 120.46322 Kcal/mol
E(PM7) = 62.59465 Kcal/mol
E(ωB97X-V/def2-TZVP) = -14776.329552213820 Hartree
E(GFN1-xTB) = -208.694121062031 Hartree
E(GFN2-xTB) = -205.328599452042 Hartree
E(GFN-FF) = -24.579821293631 Hartree

Coordinates:

C	2.359114	0.733360	1.773633
C	2.536246	1.215545	3.135302
C	1.314750	1.077448	3.773856
C	0.390958	0.510593	2.802857
C	-0.925381	0.050007	3.047678
C	-1.848514	-0.195317	2.006695
C	-3.153475	-0.797417	2.196164
H	-3.522439	-1.214840	3.138321
C	-3.793725	-0.748899	0.982776
H	-4.792785	-1.119092	0.731716
C	-2.881089	-0.114770	0.051791
C	-3.210281	0.231451	-1.277682
C	-2.249946	0.731860	-2.190717
C	-2.511530	1.405753	-3.453649
C	-1.290668	1.555846	-4.091156
C	-0.282914	0.972227	-3.217761
C	1.083053	0.751937	-3.519772
C	2.045689	0.476858	-2.524219
C	3.423518	0.119616	-2.797380
H	3.838681	-0.068949	-3.792575
C	4.065153	0.057304	-1.585273
H	5.112088	-0.193606	-1.387667
C	3.079433	0.378705	-0.571765
C	3.370374	0.539397	0.801229
C	-1.350246	-0.247657	4.438849
C	-2.472203	0.375669	5.019852
H	-3.032905	1.120820	4.436157
C	-2.865636	0.097170	6.336196
H	-3.733541	0.619578	6.759272
C	-2.137771	-0.840004	7.099883
C	-1.022024	-1.487108	6.522329
H	-0.473289	-2.221510	7.129275
C	-0.635005	-1.188342	5.218061
H	0.240177	-1.690804	4.779369
C	-3.534419	-0.554755	9.031547
H	-4.475975	-0.770485	8.475390
H	-3.390819	0.551798	9.031429
C	-3.612000	-1.084040	10.455054
H	-3.753603	-2.186365	10.415468
H	-4.531935	-0.668659	10.921834
C	-2.387020	-0.746294	11.310657
H	-1.481118	-1.133487	10.798519
H	-2.265096	0.359385	11.348456
C	-2.470959	-1.308925	12.729129
H	-1.571977	-1.052508	13.324705
H	-2.559581	-2.415428	12.718593
H	-3.355346	-0.913488	13.271758
C	-4.601806	0.000301	-1.737689
C	-5.713155	0.589475	-1.090726
H	-5.542307	1.261724	-0.236987
C	-7.012552	0.364347	-1.543612
H	-7.878313	0.837212	-1.058148
C	-7.251083	-0.477004	-2.654389
C	-6.153131	-1.090760	-3.295336
H	-6.298257	-1.775989	-4.140700
C	-4.853165	-0.841430	-2.840662
H	-4.003792	-1.321760	-3.349361
C	-8.949237	-1.341556	-4.176525
H	-8.098873	-1.433278	-4.884966
H	-9.707778	-0.693643	-4.664917
C	-9.572792	-2.704966	-3.884821
H	-10.027456	-3.040277	-4.842896
H	-10.421590	-2.557740	-3.181053
C	-8.648855	-3.813225	-3.354253
H	-7.737473	-3.869646	-3.991268
H	-9.169300	-4.783666	-3.504183
C	-8.252662	-3.696405	-1.879435
H	-7.692419	-4.594266	-1.548937
H	-9.151327	-3.607027	-1.234215
H	-7.610846	-2.817249	-1.678795
C	1.518604	0.760707	-4.937818
C	0.922888	-0.116045	-5.867368
H	0.158154	-0.826145	-5.518104
C	1.269797	-0.092876	-7.222705
H	0.779155	-0.790831	-7.913741
C	2.226982	0.835761	-7.684447
C	2.859908	1.692610	-6.756791
H	3.609962	2.403865	-7.131628
C	2.515732	1.647477	-5.406189
H	2.990441	2.343136	-4.698480
C	1.835952	0.361412	-10.016691
H	1.744054	-0.731855	-9.824127
H	2.458870	0.480148	-10.926776
C	0.457785	0.987927	-10.239253
H	-0.044299	0.363290	-11.010211
H	-0.155325	0.882758	-9.317945
C	0.452717	2.455643	-10.692439
H	-0.577055	2.701201	-11.030842
H	1.096429	2.560918	-11.594839
C	0.882907	3.469141	-9.627174
H	0.726723	4.508750	-9.979420
H	1.950704	3.354544	-9.359852
H	0.297852	3.338653	-8.692493
C	4.787859	0.445595	1.231717
C	5.179636	-0.523962	2.176585
H	4.420515	-1.207422	2.586042
C	6.508035	-0.636615	2.605845
H	6.772090	-1.408498	3.340192
C	7.483474	0.244888	2.093317
C	7.106988	1.217064	1.139140
H	7.880864	1.897185	0.754942
C	5.783076	1.307559	0.712530
H	5.495346	2.080843	-0.014912
C	9.239216	-0.699701	3.431619
H	9.057074	-1.736119	3.063512
H	8.651064	-0.572248	4.371410
C	10.723045	-0.484159	3.697431
H	11.078176	-1.374785	4.258755
H	11.257679	-0.499585	2.722336
C	11.088837	0.782847	4.485594
H	12.158809	0.706487	4.777052
H	10.520205	0.783440	5.442908
C	10.862701	2.106926	3.750845
H	11.217437	2.963670	4.358960
H	9.793604	2.270758	3.515893
H	11.413460	2.127191	2.787396
N	1.034636	0.393426	1.587401
N	-1.687667	0.168864	0.685203
N	-0.888258	0.560739	-2.047863
N	1.849331	0.584392	-1.162650
O	-2.432046	-1.183855	8.380597
O	-8.556663	-0.636504	-2.994825
O	2.608541	0.978949	-8.982326
O	8.794246	0.236881	2.450900
Cu	0.077876	0.418277	-0.235148
Br	4.022101	2.085880	3.881806
Br	0.945913	1.733645	5.492843
Br	-4.117560	2.165740	-4.059117
Br	-1.044428	2.549266	-5.666908

Conformation 22.
Multiplicity: 2
Charge: 0
E(B97-3c) = -14780.093948277321 Hartree
E(M06/def2-TZVP) = -14775.723520496045 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -14773.095567572689 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -14773.632629499658 Hartree
E(PBEh-3c) = -14765.502887779823 Hartree
E(PM6) = 120.13182 Kcal/mol
E(PM7) = 62.90533 Kcal/mol
E(ωB97X-V/def2-TZVP) = -14776.332872161749 Hartree
E(GFN1-xTB) = -208.695592316248 Hartree
E(GFN2-xTB) = -205.329799481308 Hartree
E(GFN-FF) = -24.581525029679 Hartree

Coordinates:

C	-2.818711	0.513739	0.166278
C	-3.747349	1.440949	0.795531
C	-2.985126	2.431255	1.393125
C	-1.590771	2.111196	1.126792
C	-0.463599	2.922350	1.402027
C	0.855760	2.417889	1.385240
C	2.044847	3.235933	1.521139
H	2.055207	4.329954	1.552398
C	3.113566	2.376506	1.582513
H	4.175479	2.625387	1.674952
C	2.577591	1.033022	1.485691
C	3.346816	-0.143048	1.629136
C	2.810679	-1.434821	1.407757
C	3.394577	-2.704343	1.814960
C	2.623643	-3.703913	1.244616
C	1.570015	-3.045943	0.486146
C	0.640876	-3.658462	-0.388721
C	-0.518286	-2.996056	-0.850825
C	-1.417021	-3.530055	-1.855521
H	-1.246294	-4.447133	-2.428115
C	-2.476661	-2.661791	-1.942764
H	-3.348733	-2.724835	-2.601273
C	-2.227389	-1.598987	-0.989008
C	-3.144789	-0.568709	-0.686877
C	-0.650914	4.372776	1.659887
C	-0.201079	4.977794	2.849996

H	0.280348	4.354899	3.618467
C	-0.388489	6.345742	3.092968
H	-0.042788	6.775146	4.042371
C	-1.025835	7.147158	2.121974
C	-1.463283	6.556667	0.914859
H	-1.948286	7.198914	0.165768
C	-1.283217	5.193077	0.695033
H	-1.635046	4.740256	-0.244111
C	-0.856424	9.138026	3.453693
H	0.246524	9.045928	3.585500
H	-1.341622	8.650123	4.332137
C	-1.271195	10.597805	3.355432
H	-0.770160	11.048968	2.471011
H	-0.867073	11.126879	4.246134
C	-2.785706	10.807293	3.259557
H	-3.167708	10.229011	2.392128
H	-3.270553	10.363727	4.157937
C	-3.182701	12.277318	3.127986
H	-4.282543	12.399230	3.063702
H	-2.742872	12.733337	2.216406
H	-2.830397	12.872894	3.996396
C	4.783928	0.002240	1.972885
C	5.205534	0.653271	3.155789
H	4.448399	1.041195	3.853109
C	6.559318	0.773541	3.467437
H	6.891289	1.256520	4.397772
C	7.543365	0.256879	2.594747
C	7.139099	-0.375879	1.399272
H	7.876070	-0.776104	0.690947
C	5.775455	-0.502628	1.107669
H	5.467961	-1.005325	0.178256
C	9.902650	0.013642	2.141111
H	9.708032	-1.005137	1.737237
H	10.782926	-0.063199	2.812197
C	10.194018	1.001636	1.009446
H	9.279929	1.137432	0.391328
H	10.939111	0.509570	0.346621
C	10.733616	2.371540	1.447010
H	11.093163	2.903285	0.539621
H	11.636689	2.217157	2.079821
C	9.730439	3.262155	2.186299
H	10.162566	4.262023	2.393790
H	9.418609	2.814019	3.149180
H	8.811120	3.412910	1.582331
C	0.902534	-5.028572	-0.899532
C	2.080818	-5.307988	-1.632017
H	2.805190	-4.499227	-1.811327
C	2.333376	-6.583917	-2.131064
H	3.244897	-6.804600	-2.704994
C	1.415720	-7.633582	-1.899809
C	0.233817	-7.372516	-1.174768
H	-0.495266	-8.168278	-0.973882
C	-0.012849	-6.079252	-0.692853
H	-0.928221	-5.884736	-0.114409
C	0.869985	-9.949380	-2.220198
H	-0.132835	-9.709718	-2.647530
H	0.732179	-10.127606	-1.128425
C	1.451699	-11.187335	-2.889359
H	2.487281	-11.335515	-2.511841
H	0.861236	-12.052740	-2.519222
C	1.438723	-11.193081	-4.425685
H	0.398732	-11.000298	-4.773746
H	1.678297	-12.223935	-4.765620
C	2.399226	-10.208456	-5.098241
H	2.376673	-10.322771	-6.201042
H	3.443668	-10.380328	-4.764000
H	2.149799	-9.158141	-4.854600
C	-4.478291	-0.603759	-1.338772
C	-4.895046	0.468320	-2.153182
H	-4.217064	1.323003	-2.297541
C	-6.147995	0.471723	-2.779169
H	-6.431422	1.324441	-3.409620
C	-7.026901	-0.614981	-2.585171
C	-6.618650	-1.701741	-1.779101
H	-7.318801	-2.537747	-1.637693
C	-5.362348	-1.696531	-1.175038
H	-5.062405	-2.537189	-0.532104
C	-8.758734	0.366305	-3.928387
H	-8.101353	0.487953	-4.820594
H	-8.718053	1.321071	-3.352095
C	-10.188139	0.065085	-4.358201
H	-10.434793	0.786855	-5.166130
H	-10.207895	-0.943070	-4.827458
C	-11.255827	0.161946	-3.257556
H	-12.253969	0.124414	-3.745294
H	-11.192347	1.169653	-2.788229
C	-11.186582	-0.916814	-2.173040
H	-12.029652	-0.817161	-1.459591
H	-10.241345	-0.863634	-1.599947
H	-11.240521	-1.932524	-2.617467
N	-1.528005	0.906504	0.455631
N	1.208586	1.085281	1.319567
N	1.668212	-1.681731	0.674057
N	-1.009365	-1.799043	-0.371351
O	-1.257422	8.479080	2.253772
O	8.832045	0.408958	3.003127
O	1.754284	-8.845969	-2.412200
O	-8.270896	-0.707036	-3.123930
Cu	0.087205	-0.369818	0.512846
Br	-5.605160	1.273786	1.002927
Br	-3.684734	3.769796	2.506752
Br	4.774309	-3.013785	3.049047
Br	2.837798	-5.533464	1.610992

Conformation 29.
Multiplicity: 2
Charge: 0
E(B97-3c) = -14780.093552819184 Hartree
E(M06/def2-TZVP) = -14775.722412020570 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -14773.094680285094 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -14773.631566514114 Hartree
E(PBEh-3c) = -14765.501629592944 Hartree
E(PM6) = 115.56808 Kcal/mol
E(PM7) = 58.46810 Kcal/mol
E(ωB97X-V/def2-TZVP) = -14776.331145231081 Hartree
E(GFN1-xTB) = -208.696403560423 Hartree
E(GFN2-xTB) = -205.332114814830 Hartree
E(GFN-FF) = -24.581590397895 Hartree

Coordinates:

C	2.194569	1.058225	-1.465942
C	2.571554	2.042119	-2.469382
C	1.560997	2.988848	-2.505240
C	0.567520	2.585448	-1.521455
C	-0.557107	3.331114	-1.092877
C	-1.617358	2.751198	-0.361138
C	-2.713049	3.500239	0.222765
H	-2.789536	4.591991	0.239112
C	-3.588360	2.581393	0.746385
H	-4.527330	2.767276	1.277498
C	-3.029732	1.271021	0.478746
C	-3.689598	0.053668	0.752740
C	-3.068697	-1.206138	0.570385
C	-3.727388	-2.501849	0.497552
C	-2.728197	-3.461429	0.486137
C	-1.459610	-2.752337	0.558149
C	-0.175687	-3.319527	0.743596
C	1.013638	-2.592309	0.512882
C	2.341941	-3.075467	0.834671
H	2.559909	-4.004066	1.371546
C	3.230310	-2.143831	0.357709
H	4.322736	-2.156956	0.424936
C	2.445081	-1.093393	-0.260031
C	2.991108	-0.006927	-0.979266
C	-0.611163	4.791956	-1.354419
C	-1.675518	5.378420	-2.067058
H	-2.473974	4.733793	-2.463739
C	-1.719803	6.757529	-2.315194
H	-2.556361	7.172513	-2.892400
C	-0.688073	7.588730	-1.829499
C	0.375136	7.015815	-1.095782
H	1.164579	7.680398	-0.716294
C	0.412221	5.641687	-0.870563
H	1.248417	5.203711	-0.305007
C	-1.664839	9.576322	-2.756963
H	-2.648529	9.416489	-2.257821
H	-1.728956	9.127234	-3.776449
C	-1.335465	11.058377	-2.845802
H	-1.279246	11.471229	-1.814693
H	-2.192307	11.567699	-3.338810
C	-0.036446	11.360802	-3.599379
H	0.791434	10.803360	-3.112844
H	-0.112574	10.951220	-4.631543
C	0.294064	12.851868	-3.654581
H	1.238051	13.041277	-4.203811
H	0.410018	13.276483	-2.635468
H	-0.508667	13.428104	-4.161147
C	-5.067861	0.104278	1.300352
C	-6.128821	0.707625	0.595455
H	-5.930693	1.156416	-0.389282
C	-7.437318	0.697500	1.093876
H	-8.239507	1.144885	0.492881
C	-7.711144	0.091800	2.338872
C	-6.646990	-0.475661	3.075074
H	-6.875282	-0.929261	4.050207
C	-5.353274	-0.477350	2.557565
H	-4.537271	-0.944547	3.129183
C	-10.133359	0.284968	2.193256
H	-9.972069	1.080293	1.433738
H	-10.840783	0.693526	2.943226
C	-10.720061	-0.976740	1.562565
H	-11.725052	-0.712867	1.162008

H	-10.898261	-1.717264	2.373240
C	-9.878271	-1.623912	0.456805
H	-8.873186	-1.876538	0.856354
H	-9.698523	-0.883230	-0.353433
C	-10.527936	-2.879869	-0.124761
H	-9.899689	-3.332776	-0.917644
H	-11.520353	-2.656073	-0.569637
H	-10.684768	-3.651104	0.658147
C	-0.053929	-4.704807	1.263017
C	0.655587	-5.699789	0.561057
H	1.106526	-5.450376	-0.410939
C	0.770210	-7.005904	1.055605
H	1.317971	-7.753561	0.466653
C	0.176569	-7.342910	2.291372
C	-0.522443	-6.349034	3.012866
H	-0.970841	-6.626722	3.977532
C	-0.639091	-5.058083	2.502142
H	-1.192090	-4.294745	3.069897
C	0.947146	-9.626220	2.240571
H	0.741261	-9.655259	1.145992
H	0.532393	-10.560641	2.671089
C	2.446783	-9.540972	2.517979
H	2.840616	-8.570344	2.146235
H	2.598585	-9.532472	3.619011
C	3.230323	-10.694109	1.883979
H	3.065041	-10.689362	0.783266
H	2.816182	-11.662557	2.243662
C	4.729796	-10.635020	2.177320
H	5.273031	-11.477580	1.704540
H	4.928251	-10.677634	3.268405
H	5.176917	-9.692554	1.798227
C	4.462405	0.036450	-1.170458
C	5.206582	1.132860	-0.688998
H	4.678905	1.954306	-0.181258
C	6.597603	1.197608	-0.833324
H	7.136078	2.066639	-0.433466
C	7.283080	0.151710	-1.488385
C	6.549203	-0.952929	-1.976336
H	7.097319	-1.753580	-2.493577
C	5.165524	-1.009515	-1.812903
H	4.603182	-1.866020	-2.213029
C	9.467184	1.122659	-1.145555
H	9.045849	2.130891	-1.357898
H	10.415875	1.038712	-1.714769
C	9.738787	0.949923	0.350277
H	10.281958	1.862930	0.678876
H	8.775138	0.954321	0.904681
C	10.555378	-0.291738	0.738341
H	10.858119	-0.182978	1.802292
H	11.505406	-0.294556	0.157511
C	9.833826	-1.630317	0.556233
H	10.452225	-2.470964	0.930961
H	9.595576	-1.824414	-0.507178
H	8.874121	-1.645260	1.114352
N	0.944542	1.375036	-0.974657
N	-1.810432	1.400601	-0.155092
N	-1.702945	-1.393859	0.523261
N	1.099859	-1.364538	-0.111299
O	-0.632705	8.933834	-2.011162
O	-8.936251	0.013273	2.925984
O	0.205882	-8.577514	2.861861
O	8.624925	0.113444	-1.709441
Cu	-0.365691	0.006870	-0.173384
Br	4.004753	1.984888	-3.679851
Br	1.460276	4.373838	-3.767716
Br	-5.547937	-2.877744	0.228046
Br	-3.027637	-5.291639	0.199322

Conformation 32.
Multiplicity: 2
Charge: 0
E(B97-3c) = -14780.098371216211 Hartree
E(M06/def2-TZVP) = -14775.728183140178 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -14773.099714960432 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -14773.637249647230 Hartree
E(PBEh-3c) = -14765.507380490557 Hartree
E(PM6) = 120.04579 Kcal/mol
E(PM7) = 62.51227 Kcal/mol
E(ωB97X-V/def2-TZVP) = -14776.337313630278 Hartree
E(GFN1-xTB) = -208.695118121392 Hartree
E(GFN2-xTB) = -205.330908527077 Hartree
E(GFN-FF) = -24.581469969634 Hartree

Coordinates:

C	-0.445202	0.578585	3.041472
C	-1.344836	0.193517	4.118420
C	-2.051787	-0.913082	3.676807
C	-1.581086	-1.206746	2.331692
C	-1.897542	-2.343089	1.548287
C	-1.640932	-2.401632	0.160212
C	-1.814537	-3.588553	-0.653855
H	-2.065066	-4.582666	-0.270564
C	-1.588636	-3.214474	-1.955255
H	-1.617707	-3.840452	-2.852707
C	-1.278530	-1.798648	-1.936703
C	-1.100604	-1.007035	-3.092911
C	-0.682026	0.344157	-3.031340
C	-0.765471	1.334368	-4.094772
C	-0.087899	2.458649	-3.652576
C	0.413558	2.154346	-2.320563
C	1.301421	2.939274	-1.545840
C	1.498313	2.720646	-0.164180
C	2.496991	3.400935	0.636426
H	3.260971	4.080532	0.245624
C	2.297449	3.009773	1.937131
H	2.865079	3.304279	2.825367
C	1.173720	2.093748	1.932180
C	0.573589	1.561079	3.094719
C	-2.466294	-3.549153	2.201476
C	-3.697059	-4.099998	1.793062
H	-4.261786	-3.608602	0.986944
C	-4.234988	-5.234999	2.415631
H	-5.206861	-5.621401	2.081759
C	-3.527422	-5.856953	3.466308
C	-2.281943	-5.326529	3.872088
H	-1.740152	-5.830822	4.685094
C	-1.767897	-4.189685	3.253031
H	-0.801332	-3.778912	3.581414
C	-5.210480	-7.538923	3.790486
H	-5.191336	-7.874132	2.727656
H	-6.019283	-6.776298	3.887387
C	-5.466039	-8.710256	4.726143
H	-4.639446	-9.444711	4.607253
H	-6.391101	-9.223656	4.383772
C	-5.598266	-8.308407	6.198427
H	-4.684022	-7.752873	6.495716
H	-6.439416	-7.586960	6.303003
C	-5.816048	-9.499239	7.131021
H	-5.908956	-9.178761	8.188044
H	-4.970315	-10.216055	7.073295
H	-6.738921	-10.058518	6.869111
C	-1.311160	-1.646025	-4.416660
C	-0.261251	-1.692817	-5.355584
H	0.711055	-1.250004	-5.091739
C	-0.426235	-2.287323	-6.613042
H	0.418622	-2.307045	-7.313621
C	-1.674207	-2.845650	-6.962382
C	-2.734056	-2.811670	-6.028405
H	-3.700673	-3.246262	-6.321485
C	-2.549563	-2.229018	-4.775459
H	-3.386820	-2.190178	-4.063056
C	-0.924228	-3.502735	-9.146603
H	-0.044313	-4.050789	-8.736605
H	-0.579857	-2.477369	-9.414621
C	-1.492638	-4.213469	-10.367486
H	-0.692860	-4.236706	-11.140076
H	-2.313399	-3.591344	-10.783179
C	-2.010578	-5.633678	-10.097159
H	-2.472690	-6.019717	-11.030600
H	-2.830319	-5.571670	-9.350655
C	-0.944304	-6.616344	-9.609107
H	-1.363806	-7.634968	-9.486334
H	-0.525710	-6.319279	-8.625475
H	-0.097313	-6.689252	-10.323977
C	2.111407	3.993395	-2.207443
C	2.057261	5.345158	-1.792587
H	1.381626	5.627055	-0.971537
C	2.813266	6.325294	-2.433887
H	2.758397	7.380931	-2.131053
C	3.665953	5.980052	-3.506563
C	3.749667	4.632651	-3.917581
H	4.412832	4.331521	-4.738878
C	2.972484	3.662226	-3.272634
H	3.033649	2.614515	-3.603690
C	5.216046	6.729021	-5.179533
H	4.632666	6.240123	-5.995341
H	6.019372	6.020789	-4.870788
C	5.807179	8.045456	-5.659321
H	6.371588	8.506737	-4.819445
H	6.556019	7.814449	-6.448233
C	4.766112	9.034474	-6.192926
H	4.007641	9.210563	-5.401271
H	4.218065	8.562215	-7.038775
C	5.372786	10.362669	-6.644084
H	4.597152	11.058982	-7.021183
H	6.114103	10.216225	-7.457739
H	5.898257	10.869961	-5.808091
C	1.080634	2.013802	4.414497
C	1.607866	1.074454	5.333130
H	1.631845	0.010109	5.054942
C	2.095543	1.475437	6.574401
H	2.513212	0.750314	7.287569

C	2.059938	2.838309	6.946705
C	1.540995	3.789584	6.042933
H	1.492641	4.854055	6.306990
C	1.067672	3.371363	4.791211
H	0.645684	4.114661	4.098638
C	2.530436	4.486283	8.629487
H	1.487276	4.882594	8.608336
H	3.137723	5.111808	7.934659
C	3.098808	4.555920	10.040519
H	4.089491	4.050446	10.041906
H	3.298830	5.628548	10.250071
C	2.208276	3.985481	11.154906
H	1.216432	4.489811	11.111752
H	2.649265	4.284179	12.130600
C	2.016209	2.466642	11.135442
H	1.421997	2.130501	12.009239
H	2.993402	1.941471	11.170775
H	1.500128	2.128316	10.216699
N	-0.673705	-0.237830	1.952833
N	-1.270145	-1.337256	-0.635950
N	-0.034541	0.902982	-1.948362
N	0.735254	1.897188	0.638176
O	-3.955048	-6.957498	4.137530
O	-1.949439	-3.429336	-8.157703
O	4.359544	7.002080	-4.071848
O	2.543800	3.131351	8.181970
Cu	-0.303969	0.302555	0.001652
Br	-1.702900	1.099403	5.722250
Br	-3.486735	-1.685179	4.607027
Br	-1.766810	1.264511	-5.680514
Br	-0.066702	4.100124	-4.561774

Conformation 6.
Multiplicity: 2
Charge: 0
E(B97-3c) = -14780.096269367965 Hartree
E(M06/def2-TZVP) = -14775.725834511941 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -14773.097758140699 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -14773.634955911630 Hartree
E(PBEh-3c) = -14765.505086378176 Hartree
E(PM6) = 121.47409 Kcal/mol
E(PM7) = 64.17224 Kcal/mol
E(ωB97X-V/def2-TZVP) = -14776.334985168956 Hartree
E(GFN1-xTB) = -208.694535215524 Hartree
E(GFN2-xTB) = -205.329151590731 Hartree
E(GFN-FF) = -24.580649502302 Hartree

Coordinates:

C	-1.662008	0.684668	-2.522059
C	-1.782150	0.321324	-3.926048
C	-0.951901	-0.768176	-4.132726
C	-0.322142	-1.069150	-2.855944
C	0.487802	-2.189858	-2.549108
C	1.311791	-2.236329	-1.402325
C	2.061084	-3.402581	-0.977781
H	1.988372	-4.396333	-1.430712
C	2.838383	-3.010660	0.083883
H	3.530475	-3.618532	0.675140
C	2.561665	-1.605810	0.310648
C	3.246025	-0.799387	1.247500
C	2.846363	0.526237	1.543928
C	3.619816	1.537083	2.249188
C	2.771575	2.608622	2.475434
C	1.480388	2.254216	1.905398
C	0.268554	2.977194	2.028039
C	-0.841422	2.742808	1.186208
C	-2.138865	3.369157	1.347919
H	-2.430315	4.005812	2.189221
C	-2.898039	2.995202	0.266922
H	-3.935760	3.264074	0.045499
C	-2.065711	2.137844	-0.553907
C	-2.444187	1.631827	-1.817421
C	0.438023	-3.388470	-3.423296
C	1.596893	-3.918125	-4.024837
H	2.561231	-3.413916	-3.863514
C	1.542062	-5.047062	-4.854086
H	2.464709	-5.416703	-5.320190
C	0.304463	-5.683983	-5.086578
C	-0.863002	-5.173662	-4.475207
H	-1.816315	-5.689322	-4.659977
C	-0.793888	-4.043065	-3.664702
H	-1.709185	-3.648463	-3.198524
C	1.275111	-7.350037	-6.517077
H	2.020415	-7.674028	-5.754352
H	1.766039	-6.582782	-7.161636
C	0.805137	-8.528811	-7.354973
H	0.316474	-9.268384	-6.683476
H	1.706019	-9.031692	-7.769889
C	-0.151312	-8.141418	-8.487327
H	-1.016534	-7.600924	-8.049070
H	0.356609	-7.410668	-9.155778
C	-0.636929	-9.340382	-9.301269
H	-1.327916	-9.031781	-10.111121
H	-1.177143	-10.068876	-8.661122
H	0.210332	-9.881760	-9.772427
C	4.385609	-1.404111	1.982482
C	5.507521	-1.925427	1.308343
H	5.552345	-1.856042	0.211320
C	6.582854	-2.494439	2.005062
H	7.447880	-2.870272	1.443374
C	6.542439	-2.566467	3.413621
C	5.415504	-2.062518	4.101673
H	5.398890	-2.134056	5.198707
C	4.361876	-1.486859	3.395492
H	3.491336	-1.090978	3.939759
C	8.686784	-3.636611	3.556741
H	9.195826	-2.834861	2.972820
H	8.390595	-4.435830	2.836235
C	9.625642	-4.196884	4.616375
H	9.821308	-3.401003	5.368207
H	10.595644	-4.386980	4.108893
C	9.163683	-5.485886	5.313177
H	10.027953	-5.898147	5.877660
H	8.927946	-6.246654	4.534954
C	7.972367	-5.332997	6.262783
H	7.744506	-6.291829	6.771164
H	7.061634	-4.999458	5.729790
H	8.183952	-4.578419	7.048908
C	0.125260	3.980799	3.112257
C	0.315807	3.602076	4.456588
H	0.573600	2.556815	4.684530
C	0.185666	4.521882	5.504617
H	0.338536	4.184492	6.537972
C	-0.133720	5.866078	5.217353
C	-0.331165	6.259462	3.874442
H	-0.571224	7.312920	3.670303
C	-0.210996	5.328902	2.843471
H	-0.347113	5.650276	1.800288
C	-0.093574	6.514118	7.528827
H	0.939609	6.133315	7.700201
H	-0.798728	5.699617	7.814928
C	-0.345132	7.770347	8.351801
H	-0.171848	7.508005	9.418703
H	0.425433	8.524025	8.084015
C	-1.743510	8.380315	8.176631
H	-1.872639	8.662827	7.110513
H	-1.784293	9.328528	8.753811
C	-2.892599	7.467676	8.609955
H	-3.870406	7.980976	8.514853
H	-2.784500	7.150136	9.668783
H	-2.948876	6.548995	7.990337
C	-3.743242	2.072672	-2.384854
C	-4.741708	1.125967	-2.689913
H	-4.542102	0.060354	-2.501109
C	-5.978051	1.508906	-3.225337
H	-6.730810	0.740166	-3.442565
C	-6.234805	2.872698	-3.480644
C	-5.245825	3.834180	-3.172689
H	-5.462275	4.890991	-3.385687
C	-4.025862	3.438099	-2.626820
H	-3.254814	4.191815	-2.409137
C	-8.422270	2.437228	-4.369917
H	-8.742786	1.857799	-3.471370
H	-8.027410	1.706259	-5.113175
C	-9.598463	3.205604	-4.957075
H	-9.218192	3.848603	-5.781016
H	-10.262028	2.452637	-5.433700
C	-10.422323	4.042119	-3.966513
H	-10.766203	3.380120	-3.139752
H	-11.348201	4.371205	-4.486168
C	-9.712509	5.267621	-3.384350
H	-10.397995	5.853045	-2.738485
H	-9.353453	5.940723	-4.190587
H	-8.828572	4.984343	-2.781537
N	-0.712512	-0.123430	-1.930022
N	1.596338	-1.169744	-0.573796
N	1.586896	1.027379	1.282986
N	-0.836521	1.962124	0.048131
O	0.138143	-6.781010	-5.870231
O	7.525064	-3.098757	4.187077
O	-0.270047	6.842226	6.151904
O	-7.388768	3.354217	-4.012507
Cu	0.404257	0.420273	-0.289044
Br	-2.677865	1.238429	-5.296803
Br	-0.587671	-1.510278	-5.817484
Br	5.461044	1.556949	2.611255
Br	3.322777	4.257674	3.181745

Conformation 7.
Multiplicity: 2
Charge: 0
E(B97-3c) = -14780.094628627106 Hartree

E(M06/def2-TZVP) = -14775.723670097575 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -14773.095860625714 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -14773.633005561653 Hartree
E(PBEh-3c) = -14765.503314129095 Hartree
E(PM6) = 116.39312 Kcal/mol
E(PM7) = 59.57135 Kcal/mol
E(ωB97X-V/def2-TZVP) = -14776.332625259862 Hartree
E(GFN1-xTB) = -208.695566177722 Hartree
E(GFN2-xTB) = -205.332201832048 Hartree
E(GFN-FF) = -24.581029655396 Hartree

Coordinates:

C	1.157856	-1.896711	-1.785289
C	1.830735	-1.862423	-3.075233
C	2.444267	-0.624691	-3.176948
C	2.144159	0.098794	-1.950537
C	2.684027	1.343076	-1.543414
C	2.109609	2.116906	-0.510696
C	2.694011	3.331862	0.022953
H	3.681465	3.723252	-0.240947
C	1.784209	3.855078	0.907738
H	1.875360	4.761430	1.514659
C	0.645089	2.958544	0.917267
C	-0.553852	3.203408	1.622323
C	-1.590887	2.243936	1.715973
C	-2.963371	2.478442	2.138962
C	-3.569034	1.237433	2.248379
C	-2.566385	0.244020	1.893724
C	-2.682741	-1.162494	2.010352
C	-1.798876	-2.052390	1.360220
C	-1.798633	-3.489373	1.551267
H	-2.405204	-4.025478	2.287960
C	-0.896761	-4.009026	0.656065
H	-0.615665	-5.056895	0.511290
C	-0.345147	-2.889598	-0.081655
C	0.536064	-3.014938	-1.178819
C	3.935794	1.835488	-2.172071
C	4.006532	3.090734	-2.807911
H	3.101518	3.713611	-2.865926
C	5.191998	3.545815	-3.402052
H	5.200510	4.521304	-3.905657
C	6.351115	2.742344	-3.354693
C	6.298543	1.488590	-2.704888
H	7.213904	0.880560	-2.669147
C	5.109421	1.044793	-2.131343
H	5.076509	0.063918	-1.633706
C	7.674248	4.336936	-4.567960
H	7.448516	5.170370	-3.863047
H	6.935095	4.393563	-5.402062
C	9.093274	4.448896	-5.103516
H	9.800564	4.386432	-4.247628
H	9.214248	5.467038	-5.534141
C	9.446952	3.387622	-6.150197
H	9.269009	2.384190	-5.709461
H	8.740637	3.473472	-7.006115
C	10.886713	3.494313	-6.651710
H	11.115752	2.715244	-7.406172
H	11.612230	3.376631	-5.819796
H	11.081845	4.481663	-7.120823
C	-0.692299	4.497245	2.337359
C	-0.891728	4.518492	3.738058
H	-0.936981	3.565344	4.286014
C	-1.031396	5.720514	4.428485
H	-1.181370	5.742523	5.517390
C	-0.991286	6.951020	3.735272
C	-0.785778	6.947557	2.338386
H	-0.756700	7.885318	1.767727
C	-0.628059	5.731374	1.660424
H	-0.488520	5.736864	0.569172
C	-1.244176	9.343512	3.874038
H	-0.443388	9.471469	3.109784
H	-1.035954	10.073169	4.683053
C	-2.625575	9.602271	3.275298
H	-3.382346	9.481434	4.080396
H	-2.855642	8.822143	2.517884
C	-2.744455	10.990684	2.640375
H	-1.978122	11.096060	1.839901
H	-2.493199	11.765988	3.398394
C	-4.131838	11.268426	2.060300
H	-4.189515	12.275280	1.600463
H	-4.914479	11.212474	2.845143
H	-4.396000	10.526225	1.278616
C	-3.733532	-1.737218	2.887333
C	-4.695806	-2.642426	2.396756
H	-4.678882	-2.916082	1.331345
C	-5.700452	-3.163443	3.222935
H	-6.447247	-3.843202	2.791694
C	-5.748969	-2.796343	4.585600
C	-4.774406	-1.908775	5.094669
H	-4.820340	-1.642856	6.160450
C	-3.791317	-1.386351	4.257072
H	-3.044196	-0.687522	4.662384
C	-7.739585	-4.074244	5.036579
H	-8.121930	-4.565332	5.954951
H	-7.350868	-4.880355	4.375469
C	-8.859335	-3.278220	4.364925
H	-9.210577	-2.512765	5.088275
H	-8.445729	-2.718058	3.498320
C	-10.036101	-4.148618	3.902417
H	-10.867109	-3.478499	3.596589
H	-10.426804	-4.731072	4.766950
C	-9.705306	-5.098391	2.746616
H	-10.602825	-5.656771	2.412960
H	-8.940295	-5.851570	3.026360
H	-9.315621	-4.539985	1.869481
C	0.856819	-4.381491	-1.663040
C	2.196369	-4.839381	-1.670728
H	2.992748	-4.168862	-1.314378
C	2.518676	-6.118139	-2.118865
H	3.557281	-6.478893	-2.123801
C	1.505504	-6.983310	-2.590185
C	0.163577	-6.547016	-2.582602
H	-0.644390	-7.195306	-2.945934
C	-0.145747	-5.261970	-2.115117
H	-1.191149	-4.919653	-2.130282
C	0.947227	-9.126738	-3.516865
H	0.404711	-8.670847	-4.377466
H	0.192016	-9.341570	-2.723508
C	1.643681	-10.408913	-3.952756
H	0.898025	-10.989968	-4.536705
H	2.453454	-10.140455	-4.666282
C	2.198118	-11.294446	-2.826689
H	2.474389	-12.276046	-3.269172
H	1.376537	-11.514432	-2.107902
C	3.404657	-10.727510	-2.073586
H	3.782197	-11.453253	-1.324900
H	3.156248	-9.786187	-1.547195
H	4.238007	-10.499741	-2.770480
N	1.300916	-0.668090	-1.172775
N	0.884545	1.886373	0.081866
N	-1.413111	0.892457	1.501172
N	-0.873402	-1.707505	0.396157
O	7.549218	3.085931	-3.894710
O	-1.141975	8.065969	4.500438
O	-6.668258	-3.243688	5.482957
O	1.917388	-8.203320	-3.024896
Cu	-0.020900	0.098997	0.207915
Br	1.741337	-3.110327	-4.474067
Br	3.290800	0.006797	-4.728301
Br	-3.874081	4.111608	2.302181
Br	-5.400617	0.985946	2.572868

Conformation 9.
Multiplicity: 2
Charge: 0
E(B97-3c) = -14780.095863964851 Hartree
E(M06/def2-TZVP) = -14775.724808253648 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -14773.097230574409 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -14773.634404943105 Hartree
E(PBEh-3c) = -14765.504541605114 Hartree
E(PM6) = 119.33705 Kcal/mol
E(PM7) = 61.75105 Kcal/mol
E(ωB97X-V/def2-TZVP) = -14776.334356350009 Hartree
E(GFN1-xTB) = -208.696067752465 Hartree
E(GFN2-xTB) = -205.331254471334 Hartree
E(GFN-FF) = -24.582904181538 Hartree

Coordinates:

C	2.482075	-0.501899	1.638654
C	3.911871	-0.656653	1.416126
C	4.212143	0.014906	0.242367
C	2.965653	0.578576	-0.253902
C	2.809018	1.470002	-1.343021
C	1.555907	1.715701	-1.947196
C	1.325286	2.710416	-2.976436
H	2.063843	3.441270	-3.320453
C	0.027835	2.553930	-3.396893
H	-0.510521	3.131144	-4.155347
C	-0.534954	1.464275	-2.624042
C	-1.818410	0.915191	-2.839124
C	-2.381807	-0.059833	-1.980575
C	-3.533999	-0.906103	-2.253451
C	-3.837684	-1.565988	-1.073902
C	-2.869702	-1.125277	-0.080791
C	-2.880041	-1.415020	1.305126
C	-1.749684	-1.218566	2.129128
C	-1.749836	-1.381318	3.569641
H	-2.637191	-1.573027	4.181208
C	-0.450300	-1.233131	3.986359
H	-0.059178	-1.278498	5.007621
C	0.344356	-0.979220	2.800635
C	1.753750	-0.884225	2.791325

C	3.984916	2.224899	-1.845056	H	7.086339	-1.454882	7.589959
C	4.398353	2.144651	-3.189520	N	1.933662	0.178713	0.570536
H	3.850642	1.485026	-3.878872	N	0.397158	1.002122	-1.717270
C	5.513767	2.853625	-3.656879	N	-1.960727	-0.281061	-0.685181
H	5.816274	2.747787	-4.706889	N	-0.473634	-0.928584	1.690266
C	6.235403	3.683229	-2.772297	O	7.325915	4.414793	-3.119554
C	5.819966	3.787210	-1.425553	O	-5.043906	2.832891	-7.103535
H	6.388781	4.446002	-0.753763	O	-7.669400	-3.244699	3.746806
C	4.718692	3.064353	-0.972974	O	4.610513	-1.747564	7.621086
H	4.407454	3.144914	0.079388	Cu	-0.028373	0.000508	-0.031470
C	7.811554	4.344459	-4.458706	Br	5.132280	-1.729198	2.355350
H	7.019398	4.680388	-5.167191	Br	5.889316	-0.034702	-0.597969
H	8.063664	3.287773	-4.713766	Br	-4.355431	-1.269497	-3.902164
C	9.043447	5.230074	-4.564500	Br	-5.121276	-2.927785	-0.929391
H	8.752529	6.271992	-4.306478	C	-1.106074	-2.961684	-6.098957
H	9.356924	5.249562	-5.631312	H	-1.052378	-4.026746	-6.366573
C	10.209884	4.780650	-3.679158	C	-1.591143	-2.051473	-7.064837
H	9.853973	4.722423	-2.629033	C	-1.682599	-0.681315	-6.739978
H	10.499712	3.743206	-3.959590	H	-2.053773	0.049427	-7.470358
C	11.425121	5.702829	-3.771963	C	-1.285672	-0.241086	-5.469579
H	12.252681	5.355125	-3.121679	H	-1.340419	0.830903	-5.228636
H	11.169487	6.737623	-3.461884	C	-2.395089	-1.716155	-9.302162
H	11.816041	5.757753	-4.809839	H	-1.629397	-0.928639	-9.491966
C	-2.618340	1.428285	-3.979414	H	-3.330511	-1.198381	-8.987283
C	-2.156352	1.343848	-5.308031	C	-2.640517	-2.554614	-10.549297
H	-1.179242	0.878934	-5.506713	H	-3.013826	-1.868804	-11.341376
C	-2.934054	1.792552	-6.383800	H	-3.464884	-3.267632	-10.335856
H	-2.546393	1.683147	-7.405239	C	-1.411050	-3.325549	-11.051810
C	-4.203285	2.361526	-6.142837	H	-1.722163	-3.953195	-11.913890
C	-4.662050	2.483310	-4.812142	H	-1.090588	-4.031430	-10.256835
H	-5.646262	2.942957	-4.642195	C	-0.231524	-2.440970	-11.460867
C	-3.884402	2.018308	-3.753846	H	0.600083	-3.046364	-11.873672
H	-4.258760	2.103103	-2.722583	H	0.179057	-1.873335	-10.600542
C	-4.756546	2.582169	-8.481212	H	-0.524885	-1.703586	-12.237956
H	-3.708255	2.870936	-8.719552	C	4.405825	-2.838690	-0.193184
H	-5.421884	3.279545	-9.030160	C	4.210362	-4.109938	-0.769675
C	-5.045194	1.140554	-8.897856	H	3.220188	-4.365086	-1.176469
H	-4.355429	0.451205	-8.364019	C	5.243474	-5.052968	-0.836282
H	-4.795533	1.044837	-9.978150	H	5.047153	-6.034156	-1.287619
C	-6.492980	0.705906	-8.650358	C	6.519173	-4.728056	-0.327551
H	-7.177093	1.375562	-9.218077	C	6.726981	-3.460714	0.262342
H	-6.736614	0.866540	-7.578638	H	7.729151	-3.224682	0.648239
C	-6.753633	-0.751179	-9.031223	C	5.684485	-2.538039	0.333679
H	-7.806888	-1.041170	-8.843520	H	5.863377	-1.546270	0.774605
H	-6.109022	-1.440329	-8.446450	C	7.464883	-6.830949	-0.982885
H	-6.542376	-0.935010	-10.105652	H	7.120516	-6.699472	-2.034251
C	-4.135964	-1.885513	1.942134	H	6.692644	-7.441009	-0.455977
C	-5.306439	-1.104954	1.860006	C	8.819498	-7.522797	-0.924905
H	-5.273701	-0.149076	1.315602	H	9.560119	-6.894240	-1.465592
C	-6.506583	-1.515513	2.453938	H	9.145397	-7.545600	0.136213
H	-7.393710	-0.874478	2.370693	C	8.811343	-8.944899	-1.501027
C	-6.558090	-2.744479	3.145405	H	8.078753	-9.565206	-0.937527
C	-5.391097	-3.535957	3.239658	H	9.802866	-9.404210	-1.303326
H	-5.451941	-4.492907	3.777902	C	8.508726	-9.025482	-3.000315
C	-4.200905	-3.106651	2.654260	H	8.585804	-10.067231	-3.370982
H	-3.302948	-3.738814	2.717577	H	9.221076	-8.408379	-3.587094
C	-8.885788	-2.501515	3.677587	H	7.486712	-8.668614	-3.242542
H	-9.165052	-2.331086	2.610557	C	1.567906	1.157904	4.790236
H	-8.735373	-1.500863	4.145537	C	0.508312	1.114747	5.719502
C	-9.987698	-3.262316	4.402122	H	-0.508576	0.896486	5.360004
H	-9.633590	-3.498411	5.429698	C	0.717489	1.351620	7.082583
H	-10.833677	-2.552156	4.522706	H	-0.137701	1.309978	7.769925
C	-10.498163	-4.535413	3.709764	C	2.015338	1.650545	7.550721
H	-10.801121	-4.278538	2.669561	C	3.089400	1.676317	6.633145
H	-11.433596	-4.850118	4.221158	H	4.092703	1.913079	7.015575
C	-9.519581	-5.712611	3.687000	C	2.867856	1.426587	5.279325
H	-9.986807	-6.608734	3.230519	H	3.707843	1.477944	4.570946
H	-9.202205	-5.986192	4.714921	C	1.294727	2.082557	9.807493
H	-8.601294	-5.473930	3.117080	H	1.798281	1.984671	10.790753
C	2.478460	-1.144247	4.060894	H	0.554950	1.252047	9.739405
C	3.300361	-0.142928	4.631640	C	0.607685	3.442385	9.697636
H	3.392853	0.827625	4.121447	H	1.381659	4.234125	9.794939
C	3.988321	-0.366697	5.821871	H	0.174007	3.559859	8.680873
H	4.622836	0.410344	6.271831	C	-0.485839	3.638418	10.751750
C	3.886907	-1.613983	6.478578	H	-0.048602	3.504438	11.766490
C	3.065518	-2.621158	5.928871	H	-1.246944	2.833176	10.645466
H	2.970642	-3.601259	6.414109	C	-1.168401	5.003765	10.661312
C	2.368080	-2.374736	4.737979	H	-1.957935	5.118663	11.430697
H	1.745101	-3.170617	4.303509	H	-1.642341	5.150799	9.668645
C	4.569857	-2.988523	8.324117	H	-0.438918	5.828017	10.803013
H	4.880710	-3.818479	7.645767	N	-0.309755	1.374584	1.531900
H	3.523174	-3.197691	8.646442	N	-1.025237	0.608741	-1.146089
C	5.492644	-2.918206	9.533172	N	1.359163	-0.978071	-1.402926
H	5.217445	-2.023802	10.134262	N	1.968448	-0.370867	1.341645
H	5.251941	-3.800392	10.164329	O	-7.251755	4.859204	1.054649
C	6.999233	-2.914055	9.231496	O	-1.943864	-2.583615	-8.263996
H	7.235868	-3.791074	8.587558	O	7.594456	-5.557260	-0.357362
H	7.539411	-3.093735	10.186257	O	2.336216	1.908478	8.847152
C	7.539563	-1.636673	8.583166	Cu	0.493741	0.151973	0.084214
H	8.639888	-1.690723	8.456341	Br	0.517849	4.172629	4.455350
H	7.317570	-0.747567	9.209631	Br	-2.087846	5.022538	2.294425

Br	2.296770	-1.170526	-5.420259
Br	4.902346	-2.009659	-3.255614

AVIXIO

Conformation 1.
Multiplicity: 2
Charge: 0
E(B97-3c) = -9171.813542538888 Hartree
E(GFN1-xTB) = -378.652543788501 Hartree
E(GFN2-xTB) = -362.172746393175 Hartree
E(GFN-FF) = -35.192734101492 Hartree
E(M06/def2-TZVP) = -9172.854485914644 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -9169.270673509563 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -9169.509589829700 Hartree
E(PBEh-3c) = -9158.825362182719 Hartree
E(PM6) = -561.13899 Kcal/mol
E(PM7) = -673.07934 Kcal/mol
E(ωB97X-V/def2-TZVP) = -9174.414034021638 Hartree

Coordinates:

Cu	0.773103	-0.820359	1.498124
C	0.356433	2.532813	2.234563
C	0.707611	2.188497	0.915103
C	0.807459	3.143396	-0.171716
H	0.610731	4.217319	-0.095994
C	1.142574	2.427847	-1.290356
H	1.280923	2.805254	-2.307541
C	1.251429	1.039835	-0.887644
C	1.587196	-0.012038	-1.762578
C	1.684298	-1.361394	-1.371813
C	2.176974	-2.417817	-2.233432
H	2.538641	-2.275885	-3.257430
C	2.136908	-3.578966	-1.506630
H	2.461196	-4.580005	-1.814136
C	1.595561	-3.229282	-0.206981
C	0.085377	3.967795	2.521362
C	-1.214558	4.420067	2.816796
C	-1.489462	5.777826	2.985717
C	-0.496156	6.768226	2.843416
C	0.816564	6.314737	2.582755
C	1.087351	4.952613	2.407884
C	-0.539457	8.995526	1.801057
H	0.389441	8.646546	1.316635
H	-0.361409	10.034037	2.153663
C	-1.693491	9.016095	0.771659
H	-2.544706	9.609796	1.170466
H	-1.364127	9.539963	-0.151087
C	-1.837999	7.081917	-2.225628
C	-0.924753	7.755934	-3.050022
H	0.064258	8.027313	-2.654200
C	-1.284831	8.030389	-4.376451
H	-0.564245	8.530436	-5.039855
C	-2.536814	7.634504	-4.892050
C	-3.433734	6.963719	-4.029435
H	-4.411547	6.639015	-4.417896
C	-3.096703	6.681769	-2.702216
H	-3.785767	6.134299	-2.043363
C	-2.888007	7.860600	-6.336477
H	-2.674220	6.944393	-6.928109
H	-2.290473	8.680934	-6.777770
H	-3.963631	8.094490	-6.462901
C	1.794326	0.313953	-3.199253
C	2.830815	1.148087	-3.656769
C	2.967849	1.506346	-5.006333
C	2.059364	1.046225	-5.988610
C	1.033425	0.186205	-5.524872
C	0.905317	-0.166509	-4.182463
C	2.643581	2.600548	-7.853644
H	2.615965	2.533532	-8.961347
H	3.706600	2.709540	-7.568865
C	1.876279	3.844919	-7.386476
H	1.901231	3.890623	-6.277878
H	2.385074	4.767045	-7.747821
C	-1.034208	3.724439	-5.538894
C	-0.986127	4.292550	-4.259575
H	-0.644648	5.329380	-4.136511
C	-1.377976	3.519992	-3.157297
H	-1.361705	3.962891	-2.150784
C	-1.794464	2.182699	-3.315488
C	-1.838189	1.642355	-4.622216
H	-2.142617	0.594592	-4.765050
C	-1.476078	2.405104	-5.736344
H	-1.501530	1.975323	-6.747206
C	-2.154712	1.339041	-2.121808
H	-3.195321	0.960468	-2.196564
H	-2.052556	1.907692	-1.178439
H	-1.493060	0.450502	-2.061272
N	0.976383	0.914106	0.458271
N	1.349015	-1.872813	-0.137507
N	-0.805330	8.125453	2.947203
H	-1.729269	8.273518	3.362926
N	-2.251139	7.718748	0.399413
H	-2.702668	7.184816	1.153555
N	2.116388	1.343958	-7.339521
H	1.265654	1.038393	-7.817393
N	0.475011	3.768150	-7.800294
H	0.307585	3.956612	-8.798451
S	-1.363824	6.643085	-0.558924
S	-0.636075	4.749561	-6.948087
F	-2.238332	3.550741	2.886601
F	-2.775602	6.191461	3.142251
F	2.346028	4.587982	2.134293
F	1.810933	7.206597	2.450451
F	3.731804	1.629743	-2.790377
F	3.995909	2.313944	-5.351141
F	-0.134131	-0.940551	-3.826407
F	0.120869	-0.248327	-6.425719
O	-1.934304	5.311252	-0.235426
O	0.094727	6.901246	-0.439209
O	0.024920	5.981452	-6.451876
O	-1.803507	4.838470	-7.857360
C	1.334233	-4.165770	0.810130
C	0.815029	-3.828235	2.075232
C	0.467749	-4.803202	3.089341
H	0.575433	-5.887579	2.982378
C	-0.012089	-4.101183	4.164206
H	-0.360178	-4.490772	5.126627
C	0.045684	-2.698442	3.805622
C	-0.326499	-1.654034	4.672535
C	-0.184844	-0.285958	4.363348
C	-0.475540	0.793310	5.285326
H	-0.826896	0.676266	6.314181
C	-0.230516	1.962779	4.614720
H	-0.320993	2.987312	4.990579
C	0.160994	1.599168	3.269570
C	1.596333	-5.603045	0.524890
C	2.635317	-6.308609	1.165702
C	2.878630	-7.655243	0.899089
C	2.113431	-8.396101	-0.039999
C	1.063586	-7.686486	-0.663770
C	0.832938	-6.329913	-0.402999
C	2.086513	-10.532495	-1.378434
H	2.232230	-11.598619	-1.103110
H	1.007097	-10.408770	-1.585381
C	2.899296	-10.257558	-2.660583
H	2.569120	-10.966093	-3.452980
H	3.972909	-10.462697	-2.472742
C	5.020539	-7.682992	-4.214115
C	6.295820	-8.260638	-4.168256
H	6.643558	-8.730553	-3.237330
C	7.107682	-8.202489	-5.309906
H	8.114389	-8.647885	-5.278882
C	6.665174	-7.573840	-6.491404
C	5.379153	-6.987609	-6.496959
H	5.023189	-6.475204	-7.404549
C	4.554645	-7.033990	-5.368692
H	3.562285	-6.560302	-5.369080
C	7.530174	-7.539106	-7.724612
H	8.602095	-7.662971	-7.476861
H	7.255286	-8.360218	-8.421318
H	7.408172	-6.588752	-8.280878
C	-0.980806	-2.008933	5.961633
C	-0.430644	-1.700713	7.218702
C	-1.121192	-1.928598	8.418277
C	-2.423926	-2.480702	8.426026
C	-2.953320	-2.832423	7.159781
C	-2.258899	-2.603901	5.972636
C	-3.147888	-1.842723	10.720648
H	-3.791220	-2.306406	11.497636
H	-2.124621	-1.803997	11.137364
C	-3.627784	-0.412844	10.432635
H	-2.973261	0.042592	9.659984
H	-3.523075	0.218194	11.344355
C	-4.936657	0.743944	7.452280
C	-4.184565	1.764392	6.854486
H	-3.944591	2.666164	7.436005
C	-3.752278	1.602659	5.529975
H	-3.162479	2.393817	5.044594
C	-4.050222	0.431842	4.802552
C	-4.825149	-0.569707	5.432055
H	-5.056930	-1.496044	4.885771
C	-5.280395	-0.419112	6.744752
H	-5.870318	-1.207507	7.231991
C	-3.545375	0.236040	3.397259
H	-3.007211	-0.729126	3.308195
H	-4.386969	0.204377	2.673596
H	-2.858270	1.046593	3.092246
N	0.549921	-2.554428	2.530466
N	0.216163	0.226638	3.146479
N	2.446626	-9.723324	-0.230817

H	3.364405	-9.934383	0.168193
N	2.796585	-8.894509	-3.161366
H	1.865278	-8.460581	-3.136077
N	-3.181115	-2.725016	9.559518
H	-4.134678	-2.991805	9.301193
N	-4.990333	-0.437828	9.903671
H	-5.714864	-0.667663	10.598633
S	3.970356	-7.742541	-2.762513
S	-5.553645	0.981182	9.117777
F	3.415783	-5.680751	2.055405
F	3.906078	-8.287360	1.503423
F	-0.160145	-5.726995	-1.071437
F	0.304903	-8.278700	-1.630027
F	0.794202	-1.160705	7.297923
F	-0.512347	-1.597953	9.577932
F	-2.863627	-2.914375	4.812545
F	-4.203908	-3.346774	7.118765
O	3.236538	-6.459293	-2.690050
O	4.804190	-8.255231	-1.649233
O	-4.891685	2.182979	9.676443
O	-7.023382	0.832766	9.136101

Conformation 10.
Multiplicity: 2
Charge: 0
E(B97-3c) = -9171.808552998102 Hartree
E(GFN1-xTB) = -378.644547962878 Hartree
E(GFN2-xTB) = -362.162721674580 Hartree
E(GFN-FF) = -35.180488258495 Hartree
E(M06/def2-TZVP) = -9172.848934895033 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -9169.265357790482 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -9169.502476600435 Hartree
E(PBEh-3c) = -9158.819719304962 Hartree
E(PM6) = -563.75709 Kcal/mol
E(PM7) = -672.86791 Kcal/mol
E(ωB97X-V/def2-TZVP) = -9174.404364332700 Hartree

Coordinates:

Cu	-0.436716	0.775907	-0.240791
C	0.001333	-1.160341	2.589038
C	-0.853360	-1.649642	1.585809
C	-1.512295	-2.938378	1.642163
H	-1.396539	-3.671360	2.447671
C	-2.282247	-3.035104	0.512117
H	-2.925148	-3.864416	0.201321
C	-2.082632	-1.811403	-0.239236
C	-2.704510	-1.534029	-1.474826
C	-2.447913	-0.378605	-2.238825
C	-3.135605	-0.054833	-3.473641
H	-3.950861	-0.639852	-3.912020
C	-2.589742	1.110136	-3.943684
H	-2.869544	1.671387	-4.842745
C	-1.570633	1.499654	-2.987647
C	0.281426	-2.014182	3.775792
C	-0.679496	-2.265200	4.773201
C	-0.390849	-3.025955	5.915134
C	0.890888	-3.593504	6.125317
C	1.855869	-3.331674	5.115765
C	1.555408	-2.581340	3.977289
C	0.777971	-4.039509	8.570925
H	1.329429	-4.721615	9.246499
H	-0.302116	-4.255421	8.688325
C	1.054899	-2.573778	8.985311
H	0.291609	-1.898578	8.547378
H	0.985007	-2.474032	10.087154
C	5.041820	-1.839871	8.604449
C	5.519497	-0.882456	9.511668
H	5.063932	-0.805844	10.509524
C	6.581916	-0.060422	9.121181
H	6.969687	0.693705	9.823564
C	7.173800	-0.179896	7.843132
C	6.651361	-1.140767	6.949845
H	7.090705	-1.236431	5.944910
C	5.594589	-1.982482	7.322260
H	5.201959	-2.747582	6.636211
C	8.349348	0.679967	7.469394
H	9.283155	0.273359	7.913868
H	8.227891	1.713730	7.843731
H	8.499945	0.731469	6.374559
C	-3.658840	-2.538268	-2.014792
C	-3.422091	-3.213480	-3.231098
C	-4.302166	-4.176624	-3.722501
C	-5.461435	-4.570625	-3.009363
C	-5.717812	-3.875089	-1.803944
C	-4.838276	-2.892554	-1.329872
C	-7.020214	-6.473503	-2.665272
H	-7.959793	-6.001191	-2.315134
H	-6.443853	-6.752190	-1.753563
C	-7.354613	-7.740304	-3.451580
H	-7.856083	-8.465152	-2.774567
H	-8.051811	-7.496925	-4.280054
C	-3.786373	-7.889520	-2.700696
C	-3.603681	-7.444876	-1.384564
H	-4.256679	-7.829632	-0.587833
C	-2.569460	-6.536402	-1.113182
H	-2.405814	-6.199351	-0.078000
C	-1.721338	-6.063560	-2.136116
C	-1.935639	-6.535146	-3.451789
H	-1.291859	-6.168489	-4.265894
C	-2.951602	-7.450200	-3.740875
H	-3.099624	-7.827751	-4.762705
C	-0.619897	-5.076145	-1.855299
H	-0.869663	-4.081826	-2.280464
H	0.331561	-5.395741	-2.326275
H	-0.449561	-4.939422	-0.771507
N	-1.206897	-0.984011	0.430064
N	-1.513010	0.593104	-1.948999
N	1.236940	-4.356329	7.220862
H	2.237222	-4.601926	7.228317
N	2.357622	-2.047067	8.556483
H	2.424998	-1.968833	7.531096
N	-6.258796	-5.571221	-3.520180
H	-5.790836	-6.090615	-4.273557
N	-6.149190	-8.296956	-4.079087
H	-6.338274	-8.952945	-4.847979
S	3.719982	-2.928536	9.108882
S	-5.037476	-9.128274	-3.048679
F	-1.912521	-1.756505	4.649304
F	-1.364920	-3.211180	6.830880
F	2.533218	-2.372848	3.077403
F	3.102771	-3.828976	5.279567
F	-2.296145	-2.970391	-3.926363
F	-4.028227	-4.812602	-4.883112
F	-5.151957	-2.274988	-0.181918
F	-6.833374	-4.142198	-1.093280
O	3.886449	-4.201783	8.348538
O	3.596776	-2.970587	10.579587
O	-5.713822	-9.461812	-1.774037
O	-4.444864	-10.159189	-3.925082
C	-0.773970	2.652141	-3.125581
C	0.132372	3.104330	-2.146861
C	0.939336	4.300321	-2.285268
H	0.966288	4.943310	-3.171153
C	1.628014	4.450400	-1.110166
H	2.322234	5.249921	-0.831237
C	1.259681	3.332154	-0.264978
C	1.754021	3.136235	1.037627
C	1.415461	2.038310	1.851646
C	1.922342	1.838897	3.194199
H	2.582339	2.525464	3.732923
C	1.431736	0.633589	3.624547
H	1.586876	0.148218	4.594039
C	0.633613	0.096215	2.542189
C	-0.915986	3.450153	-4.374456
C	-1.496584	4.735258	-4.378038
C	-1.633738	5.473934	-5.552641
C	-1.219563	4.978054	-6.817392
C	-0.628801	3.694812	-6.803163
C	-0.506030	2.952037	-5.622233
C	-1.433502	5.357682	-9.300287
H	-1.295646	6.252959	-9.943019
H	-0.564338	4.700489	-9.488615
C	-2.730402	4.647282	-9.742538
H	-2.648199	4.389377	-10.822192
H	-3.589534	5.341563	-9.643227
C	-5.658350	2.896981	-8.334738
C	-5.808399	1.515454	-8.539322
H	-4.988128	0.830654	-8.279553
C	-7.015930	1.036260	-9.054928
H	-7.143112	-0.046372	-9.212997
C	-8.081262	1.912445	-9.365605
C	-7.901780	3.290761	-9.133805
H	-8.726263	3.987316	-9.352456
C	-6.697753	3.791915	-8.617565
H	-6.560687	4.863535	-8.414157
C	-9.369154	1.376557	-9.935086
H	-9.232250	1.055977	-10.989929
H	-9.720607	0.487793	-9.372971
H	-10.173173	2.136981	-9.918835
C	2.736517	4.114994	1.579203
C	2.433682	4.961934	2.660062
C	3.373514	5.847539	3.207352
C	4.690605	5.932872	2.696802
C	4.984233	5.084537	1.599970
C	4.043951	4.205178	1.064088
C	5.775633	7.207631	4.551704
H	6.607948	7.940167	4.606746
H	4.858091	7.746829	4.852044
C	6.028000	6.061399	5.541417
H	5.191468	5.334228	5.481642
H	6.031475	6.449635	6.585002
C	6.596807	2.780230	4.621714

C	5.695397	1.811041	5.083540
H	5.483799	1.732351	6.159423
C	5.082142	0.959992	4.152015
H	4.375101	0.192475	4.501235
C	5.340512	1.075504	2.770271
C	6.257161	2.063870	2.341984
H	6.454968	2.187393	1.266594
C	6.896985	2.906033	3.255265
H	7.599528	3.678595	2.914133
C	4.648044	0.194939	1.765019
H	4.055060	0.808001	1.054642
H	5.385737	-0.372372	1.160316
H	3.962737	-0.524456	2.249064
N	0.353331	2.522161	-0.916956
N	0.617336	0.975988	1.481998
N	-1.408931	5.792190	-7.917098
H	-2.045659	6.563236	-7.701821
N	-3.049010	3.446774	-8.984247
H	-2.270321	2.811182	-8.770647
N	5.676762	6.783495	3.162473
H	6.581894	6.566488	2.739667
N	7.259672	5.356840	5.189045
H	8.129113	5.865826	5.400474
S	-4.113052	3.516076	-7.671197
S	7.479294	3.783127	5.814476
F	-1.936691	5.270290	-3.231040
F	-2.225304	6.685793	-5.520827
F	0.026424	1.725218	-5.710430
F	-0.263243	3.086894	-7.967546
F	1.209606	4.933822	3.204118
F	2.990803	6.622884	4.246092
F	4.425734	3.393440	0.062330
F	6.245855	5.103709	1.108555
O	-3.606775	2.507175	-6.713487
O	-4.338553	4.933450	-7.300308
O	6.795260	3.635861	7.123481
O	8.934183	3.547873	5.686998

Conformation 13.
Multiplicity: 2
Charge: 0
E(B97-3c) = -9171.820368251789 Hartree
E(GFN1-xTB) = -378.662387022279 Hartree
E(GFN2-xTB) = -362.192403200733 Hartree
E(GFN-FF) = -35.202469556621 Hartree
E(M06/def2-TZVP) = -9172.860170840058 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -9169.278208466691 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -9169.516516938764 Hartree
E(PBEh-3c) = -9158.829396510075 Hartree
E(PM6) = -570.47663 Kcal/mol
E(PM7) = -683.23308 Kcal/mol
E(ωB97X-V/def2-TZVP) = -9174.418778478581 Hartree

Coordinates:

Cu	0.235209	0.090532	0.290195
C	-2.438601	1.740589	1.728977
C	-1.663302	2.451266	0.794573
C	-1.952139	3.803395	0.358241
H	-2.794531	4.408733	0.710075
C	-0.981111	4.140983	-0.550113
H	-0.862699	5.079672	-1.101680
C	-0.088006	3.004248	-0.645407
C	1.085503	2.974422	-1.420006
C	1.966057	1.873717	-1.457667
C	3.221034	1.890278	-2.178038
H	3.642115	2.761589	-2.686735
C	3.743490	0.628262	-2.096100
H	4.640368	0.235859	-2.581691
C	2.821971	-0.152258	-1.298019
C	-3.656934	2.392660	2.292348
C	-3.736725	2.858366	3.613433
C	-4.917296	3.399607	4.144988
C	-6.111887	3.457235	3.394813
C	-6.016932	2.998434	2.054962
C	-4.839223	2.472475	1.528341
C	-7.786858	4.085174	5.184139
H	-8.672791	4.754879	5.177938
H	-7.008451	4.607123	5.773300
C	-8.188133	2.779746	5.899305
H	-8.646513	3.037589	6.880255
H	-8.965505	2.251286	5.309851
C	-7.633357	-0.840440	5.900773
C	-7.165343	-1.254750	7.157383
H	-6.375906	-0.685361	7.669213
C	-7.707510	-2.408830	7.733151
H	-7.336019	-2.754525	8.709560
C	-8.706391	-3.159744	7.074367
C	-9.148508	-2.716097	5.809688
H	-9.912976	-3.297527	5.271273
C	-8.619804	-1.564057	5.215379
H	-8.944735	-1.227098	4.221132
C	-9.281069	-4.405333	7.691941
H	-8.753144	-4.676740	8.624476
H	-9.194797	-5.268519	7.001490
H	-10.359004	-4.270262	7.921624
C	1.462238	4.129694	-2.281791
C	1.581963	3.963313	-3.679857
C	2.149158	4.941289	-4.494727
C	2.625534	6.179233	-3.984466
C	2.466573	6.359602	-2.587108
C	1.909726	5.361121	-1.771674
C	4.030053	8.183492	-4.498761
H	3.548095	8.777917	-3.701346
H	4.127410	8.850351	-5.381170
C	5.441113	7.776026	-4.017204
H	5.856401	8.589403	-3.385386
H	5.368408	6.886825	-3.354980
C	6.682661	4.829913	-4.845423
C	5.775549	3.764830	-4.760590
H	4.867040	3.766879	-5.379722
C	6.064552	2.704624	-3.893843
H	5.380627	1.846764	-3.863499
C	7.223427	2.703085	-3.086380
C	8.112950	3.795132	-3.200459
H	9.025569	3.811727	-2.584519
C	7.862567	4.851082	-4.083754
H	8.563913	5.692473	-4.179117
C	7.503027	1.559670	-2.150192
H	6.636522	1.352173	-1.490267
H	8.384575	1.759181	-1.511936
H	7.695249	0.631790	-2.726609
N	-0.529507	1.981772	0.167806
N	1.759555	0.631526	-0.897792
N	-7.335871	3.942253	3.814408
H	-8.073748	3.714402	3.144641
N	-7.084107	1.852699	6.115722
H	-6.168272	2.273735	6.321512
N	3.154107	7.088211	-4.876710
H	3.427901	6.645722	-5.764397
N	6.452271	7.502111	-5.036333
H	6.741926	8.296845	-5.620598
S	-6.842960	0.540555	5.084183
S	6.397297	6.130515	-6.031306
F	-2.666848	2.780849	4.415241
F	-4.909112	3.777024	5.455506
F	-4.845679	2.021707	0.266381
F	-7.141441	3.018686	1.306963
F	1.188531	2.817152	-4.253094
F	2.293015	4.704224	-5.817046
F	1.857753	5.595045	-0.451625
F	2.893011	7.497457	-1.986983
O	-5.373341	0.323483	5.137364
O	-7.552107	0.747910	3.795148
O	5.056693	5.909919	-6.645401
O	7.565166	6.295741	-6.927972
C	2.985939	-1.530389	-1.053203
C	2.074496	-2.304046	-0.312423
C	2.188568	-3.734538	-0.114278
H	2.993880	-4.360499	-0.513343
C	1.113048	-4.114594	0.647361
H	0.852351	-5.119558	0.995635
C	0.362762	-2.909003	0.940353
C	-0.770280	-2.859845	1.774880
C	-1.455788	-1.673196	2.100646
C	-2.545023	-1.614068	3.053639
H	-2.903550	-2.458809	3.650442
C	-3.012368	-0.325210	3.048750
H	-3.834523	0.096036	3.637335
C	-2.198413	0.402941	2.096110
C	4.162746	-2.177915	-1.703077
C	5.486851	-1.842617	-1.353619
C	6.580343	-2.284138	-2.098089
C	6.439434	-3.075286	-3.268564
C	5.112980	-3.442005	-3.590688
C	4.018552	-2.991100	-2.840509
C	7.657456	-3.895719	-5.323560
H	8.617423	-4.440165	-5.452315
H	6.854614	-4.636401	-5.490816
C	7.592138	-2.795096	-6.405700
H	7.646757	-3.274715	-7.407977
H	8.473928	-2.129327	-6.318167
C	6.379510	0.826454	-6.638769
C	5.140272	1.167466	-7.203709
H	4.239442	0.590212	-6.950225
C	5.068917	2.275132	-8.055829
H	4.098253	2.558346	-8.491071
C	6.208983	3.057374	-8.344627
C	7.433373	2.699391	-7.738532
H	8.321725	3.325371	-7.913151
C	7.529912	1.588322	-6.891435
H	8.473488	1.329672	-6.390974
C	6.130485	4.238873	-9.272556

H	5.085279	4.568145	-9.422003
H	6.707746	5.093580	-8.869847
H	6.556182	3.980469	-10.265961
C	-1.308010	-4.125339	2.348475
C	-0.629459	-4.860893	3.336796
C	-1.164165	-6.026617	3.906038
C	-2.441108	-6.511161	3.533744
C	-3.112767	-5.774470	2.525916
C	-2.571379	-4.618731	1.960035
C	-2.965006	-8.033253	5.433507
H	-3.196584	-9.117174	5.517456
H	-1.937300	-7.897898	5.813775
C	-3.946953	-7.230307	6.297431
H	-3.722349	-6.148391	6.188436
H	-3.819184	-7.476943	7.375697
C	-6.339265	-5.077503	4.962962
C	-5.686016	-3.869155	5.246371
H	-5.283426	-3.690480	6.252953
C	-5.605926	-2.893720	4.246851
H	-5.139032	-1.926335	4.479701
C	-6.164817	-3.107556	2.966712
C	-6.813477	-4.336553	2.717904
H	-7.256104	-4.519172	1.726595
C	-6.911279	-5.322971	3.705851
H	-7.433893	-6.271707	3.518062
C	-6.067827	-2.042134	1.909306
H	-5.017174	-1.934293	1.568409
H	-6.692319	-2.281507	1.027680
H	-6.380440	-1.055479	2.307485
N	0.954018	-1.822676	0.332119
N	-1.237113	-0.426854	1.555653
N	7.587391	-3.424802	-3.953277
H	8.387363	-2.861953	-3.654267
N	6.407212	-1.949273	-6.346216
H	5.512811	-2.428465	-6.181451
N	-3.025878	-7.669930	4.023055
H	-3.977090	-7.779776	3.655631
N	-5.311590	-7.456645	5.818246
H	-5.706513	-8.375078	6.065630
S	6.445406	-0.511497	-5.453498
S	-6.503789	-6.305204	6.247917
F	5.720023	-1.036490	-0.305482
F	7.827537	-1.890459	-1.752947
F	2.793117	-3.318939	-3.273482
F	4.845380	-4.127107	-4.737670
F	0.575144	-4.453651	3.761375
F	-0.427996	-6.679732	4.832254
F	-3.292649	-3.964453	1.036608
F	-4.327015	-6.213526	2.127688
O	5.165425	-0.480625	-4.702358
O	7.764591	-0.431748	-4.771736
O	-6.159036	-5.663425	7.539832
O	-7.778061	-7.041205	6.069530

Conformation 14.
Multiplicity: 2
Charge: 0
E(B97-3c) = -9171.796571575876 Hartree
E(GFN1-xTB) = -378.632797383453 Hartree
E(GFN2-xTB) = -362.151388178892 Hartree
E(GFN-FF) = -35.175255388708 Hartree
E(M06/def2-TZVP) = -9172.837903378861 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -9169.256506800213 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -9169.493729390215 Hartree
E(PBEh-3c) = -9158.806131438232 Hartree
E(PM6) = -554.04840 Kcal/mol
E(PM7) = -663.36746 Kcal/mol
E(ωB97X-V/def2-TZVP) = -9174.396102721235 Hartree

Coordinates:

Cu	1.349602	-0.201096	-0.923741
C	-0.031197	2.646208	0.474123
C	-0.616008	2.132758	-0.695849
C	-1.782513	2.706783	-1.336634
H	-2.291804	3.625305	-1.029798
C	-2.104383	1.883136	-2.382257
H	-2.896851	2.028060	-3.122918
C	-1.134887	0.804508	-2.371419
C	-1.166163	-0.271553	-3.278629
C	-0.151995	-1.236458	-3.387540
C	-0.084915	-2.234237	-4.435910
H	-0.826255	-2.355680	-5.233246
C	1.083052	-2.928236	-4.250259
H	1.500056	-3.729423	-4.871341
C	1.697394	-2.385150	-3.050995
C	-0.747803	3.771494	1.139089
C	-0.718496	5.095603	0.660374
C	-1.539274	6.086082	1.205698
C	-2.457236	5.825799	2.259119
C	-2.479446	4.492926	2.735352
C	-1.631575	3.517487	2.199989
C	-4.109590	6.852407	3.876268
H	-4.794136	5.984009	3.873459
H	-4.745757	7.758197	3.831087
C	-3.339264	6.859902	5.212677
H	-2.669715	5.970441	5.270094
H	-2.681720	7.752489	5.259151
C	-3.706326	4.543236	7.704885
C	-3.039137	3.553557	6.964585
H	-3.319221	3.365632	5.919358
C	-2.039382	2.796455	7.591808
H	-1.524447	2.007857	7.021160
C	-1.692639	3.007147	8.943973
C	-2.390025	4.006093	9.660097
H	-2.151166	4.171379	10.722527
C	-3.393472	4.770760	9.055823
H	-3.960881	5.521323	9.625511
C	-0.608592	2.200627	9.604403
H	-0.484755	1.204751	9.138950
H	-0.807323	2.051610	10.683668
H	0.375749	2.709961	9.526477
C	-2.414468	-0.378765	-4.088282
C	-3.602490	-0.768714	-3.438366
C	-4.841838	-0.670502	-4.066396
C	-4.990528	-0.128831	-5.364647
C	-3.792540	0.191222	-6.042537
C	-2.543990	0.082519	-5.409348
C	-6.648501	1.148696	-6.732924
H	-7.755658	1.127332	-6.795634
H	-6.271157	0.989161	-7.764605
C	-6.158881	2.536580	-6.281971
H	-5.056258	2.574200	-6.376885
H	-6.563936	3.303313	-6.980172
C	-5.445104	3.319002	-2.370649
C	-5.585004	1.967209	-2.026959
H	-5.784952	1.220538	-2.802957
C	-5.482162	1.592164	-0.683490
H	-5.579103	0.527237	-0.421880
C	-5.236001	2.545384	0.328738
C	-5.117883	3.901656	-0.047536
H	-4.939001	4.663824	0.727656
C	-5.218402	4.297203	-1.388419
H	-5.123594	5.351577	-1.685758
C	-5.079632	2.120522	1.764029
H	-5.702980	1.234887	1.995373
H	-5.342162	2.930702	2.470722
H	-4.026192	1.840364	1.975324
N	-0.220538	0.990159	-1.358864
N	0.943069	-1.341890	-2.556968
N	-3.261267	6.851412	2.697268
H	-3.009754	7.758954	2.305468
N	-4.259922	6.933526	6.342895
H	-3.985014	7.545192	7.117312
N	-6.267701	0.035901	-5.872258
H	-6.968117	-0.185584	-5.163111
N	-6.471365	2.833634	-4.879584
H	-7.395702	3.261501	-4.736386
S	-5.003062	5.528638	6.945434
S	-5.311274	3.825911	-4.082451
F	0.085318	5.417862	-0.359689
F	-1.477611	7.351787	0.734642
F	-1.727801	2.269288	2.707928
F	-3.330235	4.129917	3.723346
F	-3.567568	-1.178322	-2.161538
F	-5.971706	-0.982519	-3.380259
F	-1.456035	0.467877	-6.087475
F	-3.843165	0.677326	-7.302255
O	-5.496156	4.789544	5.764484
O	-5.888074	6.014397	8.019891
O	-3.997116	3.377173	-4.607401
O	-5.694864	5.252305	-4.164755
C	2.863466	-2.905148	-2.457838
C	3.405091	-2.438396	-1.242827
C	4.534684	-3.055178	-0.575913
H	5.100626	-3.909725	-0.961174
C	4.720122	-2.374842	0.600079
H	5.481629	-2.545293	1.368744
C	3.712285	-1.335015	0.644076
C	3.594762	-0.402796	1.692426
C	2.693965	0.682299	1.688410
C	2.615032	1.686713	2.730901
H	3.228810	1.718383	3.635570
C	1.626114	2.562370	2.362721
H	1.280906	3.458645	2.889463
C	1.077668	2.071214	1.117987
C	3.539200	-4.054145	-3.122353
C	4.789085	-3.908312	-3.757204
C	5.424922	-4.983755	-4.376398
C	4.852786	-6.282517	-4.423012
C	3.610246	-6.423615	-3.766341
C	2.969640	-5.336614	-3.158506
C	5.019766	-8.518448	-5.574152

H	5.866926	-9.213229	-5.756833
H	4.398053	-8.984566	-4.787243
C	4.207877	-8.403921	-6.880897
H	3.875918	-9.421393	-7.186559
H	4.858989	-8.021442	-7.693110
C	2.405410	-5.901378	-8.915649
C	3.216798	-5.838719	-10.056291
H	4.308399	-5.778463	-9.941433
C	2.610240	-5.836880	-11.319886
H	3.241609	-5.787785	-12.220908
C	1.208045	-5.888178	-11.458866
C	0.420352	-5.941758	-10.287173
H	-0.676906	-5.975968	-10.375457
C	1.006121	-5.944541	-9.017171
H	0.390869	-5.969622	-8.106228
C	0.562328	-5.846851	-12.819485
H	-0.389138	-6.413743	-12.838256
H	0.323111	-4.800496	-13.107887
H	1.229540	-6.256769	-13.602498
C	4.398410	-0.615685	2.926851
C	5.351527	0.305604	3.396207
C	5.963485	0.178568	4.651892
C	5.642372	-0.887741	5.524862
C	4.723950	-1.842258	5.023320
C	4.123308	-1.710221	3.771560
C	6.497132	0.057725	7.662500
H	6.930433	-0.367455	8.591828
H	7.286754	0.679546	7.201304
C	5.300300	0.955438	8.008100
H	4.868077	1.365214	7.071298
H	5.640888	1.830574	8.606506
C	1.971854	0.389020	7.211795
C	1.273572	1.351041	6.467832
H	1.254999	2.394762	6.812561
C	0.623410	0.956204	5.289869
H	0.075921	1.698824	4.691422
C	0.679219	-0.377379	4.834036
C	1.382697	-1.322528	5.615361
H	1.454184	-2.364118	5.269140
C	2.017464	-0.954219	6.805120
H	2.579057	-1.690852	7.395646
C	0.038564	-0.785066	3.534360
H	0.777142	-1.292350	2.880935
H	-0.789292	-1.504809	3.705503
H	-0.366205	0.085636	2.986160
N	2.925691	-1.389519	-0.487293
N	1.753653	0.939790	0.712889
N	5.565392	-7.272649	-5.071884
H	6.313742	-6.874070	-5.644064
N	3.048875	-7.526109	-6.798434
H	2.487670	-7.585365	-5.939425
N	6.175154	-1.066166	6.790809
H	5.700757	-1.828409	7.280512
N	4.258381	0.176884	8.676772
H	4.489834	-0.120181	9.635190
S	3.162045	-5.909699	-7.290928
S	2.697569	0.866906	8.777124
F	5.392992	-2.712561	-3.769176
F	6.603477	-4.798392	-5.006337
F	1.771530	-5.552920	-2.597233
F	2.935023	-7.607940	-3.806315
F	5.687552	1.361934	2.642946
F	6.860673	1.117705	5.024003
F	3.204926	-2.621329	3.406668
F	4.370665	-2.866740	5.834942
O	2.264282	-5.165389	-6.379726
O	4.589466	-5.555805	-7.478155
O	2.777364	2.349113	8.801878
O	2.049294	0.122695	9.879173

Conformation 18.
Multiplicity: 2
Charge: 0
E(B97-3c) = -9171.796212722034 Hartree
E(GFN1-xTB) = -378.628962929520 Hartree
E(GFN2-xTB) = -362.148174375241 Hartree
E(GFN-FF) = -35.158265336237 Hartree
E(M06/def2-TZVP) = -9172.842458827785 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -9169.254649370218 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -9169.492385560572 Hartree
E(PBEh-3c) = -9158.808550530821 Hartree
E(PM6) = -558.81527 Kcal/mol
E(PM7) = -663.66912 Kcal/mol
E(ωB97X-V/def2-TZVP) = -9174.393694896908 Hartree

Coordinates:

Cu	-1.822881	0.274865	0.441420
C	0.771896	1.653308	2.269916
C	0.984842	0.407329	1.650135
C	2.225018	-0.334126	1.746630
H	3.088320	-0.041392	2.353328
C	2.087001	-1.439621	0.949368
H	2.824091	-2.224219	0.757937
C	0.754227	-1.384956	0.383447
C	0.246090	-2.327917	-0.534251
C	-1.062301	-2.295185	-1.049193
C	-1.607959	-3.311647	-1.927458
H	-1.062607	-4.192271	-2.282891
C	-2.912181	-2.971558	-2.172242
H	-3.652593	-3.517232	-2.768772
C	-3.156450	-1.739414	-1.445473
C	1.930601	2.276101	2.965632
C	1.970098	2.460743	4.363237
C	3.083541	3.015518	4.996011
C	4.242507	3.428415	4.283710
C	4.193056	3.253630	2.878377
C	3.072534	2.689589	2.253858
C	6.632378	4.220268	4.514195
H	7.178002	4.765575	5.307464
H	6.619728	4.871184	3.618321
C	7.421318	2.936274	4.189865
H	7.359697	2.229849	5.051195
H	6.959402	2.424207	3.323145
C	10.144032	1.631819	5.660007
C	9.408076	1.214151	6.778424
H	8.787570	1.942791	7.319564
C	9.510861	-0.119185	7.201684
H	8.940419	-0.451738	8.083030
C	10.340243	-1.038597	6.528475
C	11.084263	-0.580680	5.417117
H	11.755936	-1.278419	4.892428
C	10.994521	0.744260	4.979103
H	11.591611	1.106676	4.129227
C	10.434543	-2.475766	6.970500
H	9.916642	-3.145261	6.251051
H	9.972773	-2.631760	7.964160
H	11.488879	-2.815191	7.021104
C	1.182144	-3.371742	-1.033444
C	1.766109	-4.335485	-0.190376
C	2.765346	-5.213224	-0.632278
C	3.242194	-5.171085	-1.963721
C	2.594989	-4.257388	-2.830378
C	1.617078	-3.373327	-2.375235
C	5.396364	-6.338587	-1.607755
H	5.159612	-7.227936	-0.989617
H	5.670084	-5.521360	-0.901741
C	6.599877	-6.648545	-2.495766
H	7.477702	-6.868155	-1.850486
H	6.390855	-7.545215	-3.115508
C	6.246905	-2.988103	-2.559538
C	6.021981	-2.461302	-1.280243
H	6.632818	-2.814415	-0.436920
C	5.037083	-1.476201	-1.114637
H	4.865715	-1.040917	-0.118676
C	4.268451	-1.017063	-2.204644
C	4.518508	-1.576941	-3.478911
H	3.920802	-1.241248	-4.340038
C	5.509164	-2.544474	-3.668894
H	5.710972	-2.956824	-4.667678
C	3.204611	0.034218	-2.032267
H	2.195020	-0.422383	-2.099190
H	3.265204	0.794928	-2.836328
H	3.275062	0.545733	-1.054464
N	0.093325	-0.263856	0.840191
N	-2.021180	-1.345222	-0.768039
N	5.284665	3.974339	4.992411
H	5.155586	3.936338	6.003334
N	8.803416	3.243341	3.838909
H	9.180262	2.822775	2.984703
N	4.266272	-5.957625	-2.448930
H	4.593107	-5.626526	-3.365400
N	6.852304	-5.549148	-3.436274
H	7.426065	-5.813805	-4.247228
S	9.973262	3.317397	5.056132
S	7.608879	-4.128833	-2.806738
F	0.928373	2.084172	5.116866
F	3.097217	3.156112	6.340716
F	3.111518	2.553534	0.916949
F	5.241433	3.615271	2.102069
F	1.379860	-4.420997	1.091617
F	3.274555	-6.108376	0.239832
F	1.135519	-2.461052	-3.237942
F	3.008408	-4.204267	-4.115953
O	9.371496	4.112554	6.147913
O	11.224473	3.687085	4.372299
O	8.189228	-4.436185	-1.478398
O	8.430712	-3.636051	-3.931205
C	-4.399256	-1.080935	-1.425608
C	-4.660808	0.088551	-0.686988
C	-5.949573	0.750505	-0.660896
H	-6.844048	0.406726	-1.190312
C	-5.809263	1.855809	0.136084

H	-6.570875	2.594177	0.407385
C	-4.429999	1.878441	0.581119
C	-3.879929	2.902293	1.376229
C	-2.549406	2.907463	1.843011
C	-1.966116	3.986593	2.614028
H	-2.483393	4.903427	2.911428
C	-0.661480	3.641680	2.854719
H	0.098418	4.213587	3.397520
C	-0.450418	2.350125	2.235291
C	-5.503855	-1.649349	-2.248051
C	-6.606157	-2.307264	-1.667539
C	-7.639323	-2.828233	-2.445889
C	-7.640961	-2.745256	-3.863512
C	-6.538479	-2.071798	-4.435096
C	-5.495528	-1.566087	-3.649267
C	-8.737327	-3.671761	-5.935469
H	-9.798660	-3.792037	-6.239909
H	-8.331676	-2.839918	-6.540824
C	-7.992708	-4.979053	-6.276495
H	-8.109413	-5.186064	-7.363865
H	-8.460892	-5.826122	-5.735177
C	-5.401779	-7.240874	-4.939903
C	-4.139012	-7.321598	-5.548396
H	-3.549718	-6.407530	-5.710735
C	-3.646303	-8.576635	-5.918724
H	-2.653720	-8.648321	-6.390609
C	-4.391533	-9.755163	-5.688718
C	-5.647697	-9.639081	-5.059535
H	-6.234607	-10.547653	-4.852678
C	-6.159456	-8.390158	-4.680003
H	-7.128242	-8.296516	-4.168993
C	-3.859007	-11.096598	-6.120956
H	-4.039869	-11.260569	-7.205170
H	-2.765031	-11.171767	-5.961603
H	-4.348399	-11.926992	-5.576414
C	-4.725387	4.089529	1.675022
C	-5.071397	4.469322	2.985491
C	-5.807346	5.630465	3.263684
C	-6.241182	6.494462	2.230104
C	-5.910107	6.094791	0.911273
C	-5.178452	4.938686	0.644122
C	-6.783160	8.539734	3.546463
H	-7.583693	9.307987	3.503053
H	-6.923672	7.987048	4.493070
C	-5.406828	9.220063	3.552874
H	-4.619452	8.439555	3.618693
H	-5.293270	9.861220	4.456251
C	-2.994055	8.862174	1.153220
C	-1.926060	8.187154	1.757843
H	-1.496452	8.584719	2.688622
C	-1.431196	7.022596	1.152545
H	-0.594912	6.480648	1.618764
C	-1.991630	6.522551	-0.040642
C	-3.059951	7.238623	-0.629936
H	-3.517355	6.859781	-1.556101
C	-3.559109	8.407862	-0.049594
H	-4.390706	8.959324	-0.509741
C	-1.484379	5.253123	-0.672160
H	-2.300237	4.506235	-0.752013
H	-1.114778	5.439538	-1.701812
H	-0.665789	4.800225	-0.082253
N	-3.753733	0.783471	0.084885
N	-1.609380	1.923069	1.619597
N	-8.715060	-3.296131	-4.535426
H	-9.263365	-3.903704	-3.921974
N	-6.577230	-4.973588	-5.936779
H	-6.053199	-4.114291	-6.144155
N	-6.985803	7.647480	2.410521
H	-7.061229	8.163998	1.529570
N	-5.208044	9.946320	2.299824
H	-5.755017	10.815177	2.215771
S	-6.041864	-5.633011	-4.473567
S	-3.596524	10.379132	1.895238
F	-6.677576	-2.435960	-0.335645
F	-8.663914	-3.479556	-1.857573
F	-4.464713	-0.983311	-4.277174
F	-6.399144	-1.994974	-5.789342
F	-4.698860	3.704694	4.021492
F	-6.099069	5.907567	4.552902
F	-4.864175	4.669039	-0.635399
F	-6.286843	6.901426	-0.106144
O	-4.888891	-4.795822	-4.071943
O	-7.208756	-5.870292	-3.590893
O	-2.803952	10.625422	3.121778
O	-3.758753	11.416037	0.856219

Conformation 20.
Multiplicity: 2
Charge: 0
E(B97-3c) = -9171.798942544761 Hartree
E(GFN1-xTB) = -378.633762794353 Hartree
E(GFN2-xTB) = -362.151672108256 Hartree
E(GFN-FF) = -35.159254823016 Hartree
E(M06/def2-TZVP) = -9172.839297263821 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -9169.257329525668 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -9169.494237510464 Hartree
E(PBEh-3c) = -9158.811205236058 Hartree
E(PM6) = -563.74922 Kcal/mol
E(PM7) = -664.41659 Kcal/mol
E(ωB97X-V/def2-TZVP) = -9174.393707944870 Hartree

Coordinates:

Cu	0.012696	-0.014547	0.616745
C	2.282062	-2.498786	1.419456
C	1.768209	-2.476909	0.110257
C	2.179953	-3.387531	-0.938670
H	2.952330	-4.156922	-0.838546
C	1.425686	-3.083984	-2.041820
H	1.457199	-3.549778	-3.032155
C	0.567543	-1.976466	-1.670317
C	-0.343399	-1.360449	-2.551519
C	-1.088836	-0.208786	-2.231930
C	-2.043715	0.413895	-3.128298
H	-2.319912	0.032354	-4.116419
C	-2.524254	1.528406	-2.493110
H	-3.266111	2.247260	-2.859788
C	-1.871716	1.573241	-1.198135
C	3.349494	-3.478819	1.760378
C	4.657106	-3.046858	2.061065
C	5.659606	-3.938842	2.444257
C	5.439450	-5.340442	2.511412
C	4.122566	-5.771471	2.213270
C	3.117747	-4.865036	1.845162
C	6.312743	-7.332471	3.723754
H	7.329679	-7.732933	3.900264
H	5.721840	-8.128573	3.230194
C	5.662089	-6.982607	5.083688
H	4.563558	-6.875260	4.970718
H	5.838122	-7.805030	5.805911
C	7.918627	-4.182260	6.984154
C	8.012792	-4.344300	8.374155
H	8.023805	-5.357017	8.802008
C	8.109728	-3.203570	9.177254
H	8.194652	-3.318282	10.269251
C	8.104392	-1.905191	8.617766
C	8.004488	-1.782447	7.214697
H	8.002581	-0.779355	6.760328
C	7.922472	-2.911677	6.388233
H	7.873160	-2.814802	5.293289
C	8.193482	-0.695073	9.506386
H	8.247310	0.245721	8.927218
H	9.081108	-0.749686	10.169948
H	7.297429	-0.623065	10.155304
C	-0.530886	-1.962556	-3.899091
C	-0.178133	-1.288167	-5.083134
C	-0.380512	-1.841715	-6.355928
C	-0.967170	-3.119794	-6.520643
C	-1.311795	-3.798733	-5.320942
C	-1.102416	-3.243003	-4.058996
C	-1.187802	-3.168846	-9.042359
H	-1.343228	-3.989380	-9.767550
H	-0.202356	-2.713012	-9.262669
C	-2.301060	-2.125617	-9.277513
H	-3.251306	-2.498751	-8.830040
H	-2.051830	-1.182392	-8.752892
C	-5.174490	-2.271099	-11.087061
C	-5.827827	-1.216536	-11.743364
H	-5.350973	-0.743201	-12.614008
C	-7.091221	-0.813660	-11.293283
H	-7.619615	-0.006090	-11.823560
C	-7.709973	-1.435765	-10.186645
C	-7.038423	-2.509628	-9.564572
H	-7.517071	-3.031200	-8.720945
C	-5.781704	-2.938842	-10.010798
H	-5.280533	-3.804449	-9.554425
C	-9.041956	-0.957356	-9.670106
H	-8.900323	-0.255114	-8.819798
H	-9.661589	-1.796022	-9.295431
H	-9.616030	-0.419803	-10.449747
N	0.796643	-1.617493	-0.360000
N	-1.010405	0.505271	-1.055098
N	6.481892	-6.178726	2.846065
H	7.340306	-5.662170	3.086975
N	6.131238	-5.729540	5.691361
H	5.846257	-4.902426	5.146623
N	-1.202080	-3.755043	-7.716538
H	-1.715921	-4.630284	-7.615977
N	-2.457463	-1.827707	-10.697527
H	-2.446461	-0.846623	-10.989558
S	7.823339	-5.632534	5.949579
S	-3.525263	-2.748384	-11.626504
F	4.957424	-1.736168	2.023558

F	6.886533	-3.468284	2.763674
F	1.897454	-5.351218	1.580837
F	3.817363	-7.084785	2.272662
F	0.381318	-0.071718	-5.015626
F	-0.017762	-1.110657	-7.437424
F	-1.473891	-3.948548	-2.982443
F	-1.887377	-5.016974	-5.438608
O	8.539222	-5.313965	4.680141
O	8.179824	-6.850248	6.705775
O	-3.350168	-2.278025	-13.011615
O	-3.317741	-4.149764	-11.202989
C	-2.124713	2.565429	-0.233624
C	-1.583951	2.560049	1.065443
C	-1.870478	3.573731	2.060332
H	-2.501018	4.453306	1.893824
C	-1.215000	3.199325	3.204458
H	-1.206689	3.703213	4.176405
C	-0.516527	1.966278	2.900082
C	0.263275	1.254329	3.829187
C	0.950313	0.060824	3.532875
C	1.756298	-0.667415	4.491385
H	1.889804	-0.397374	5.543319
C	2.321190	-1.716804	3.813766
H	2.984013	-2.495549	4.205727
C	1.867292	-1.622773	2.441756
C	-3.043711	3.676829	-0.608264
C	-4.365523	3.746269	-0.125185
C	-5.228661	4.774032	-0.504407
C	-4.840382	5.803983	-1.402080
C	-3.505151	5.740606	-1.858921
C	-2.651645	4.690250	-1.496544
C	-5.727780	7.692533	-2.823025
H	-6.430879	8.526104	-2.610797
H	-4.717990	8.140783	-2.873004
C	-6.103181	7.095997	-4.196300
H	-6.049199	7.901058	-4.963273
H	-7.153965	6.741622	-4.175640
C	-6.366334	3.838549	-5.928705
C	-5.432086	3.455654	-6.904731
H	-4.359073	3.463587	-6.665567
C	-5.893643	3.051931	-8.160637
H	-5.168883	2.744699	-8.931268
C	-7.274821	3.022626	-8.459413
C	-8.186438	3.391750	-7.450118
H	-9.267182	3.355902	-7.659175
C	-7.742942	3.798251	-6.183127
H	-8.449960	4.069182	-5.386444
C	-7.745726	2.619717	-9.831947
H	-7.571107	3.438453	-10.562633
H	-7.191952	1.733377	-10.201056
H	-8.827969	2.386112	-9.844713
C	0.425581	1.815761	5.198741
C	-0.117134	1.188949	6.334045
C	0.096465	1.672205	7.633161
C	0.885717	2.822288	7.871196
C	1.413130	3.459657	6.720470
C	1.191317	2.974689	5.431451
C	1.282165	2.556868	10.318705
H	1.405266	3.256966	11.171475
H	0.347557	1.996124	10.503684
C	2.453240	1.565512	10.279017
H	2.315369	0.874694	9.421187
H	2.451155	0.933087	11.195294
C	4.833829	1.373039	7.768032
C	4.926059	0.167733	7.057510
H	5.071309	-0.775147	7.604050
C	4.824172	0.199170	5.658674
H	4.893441	-0.737489	5.085427
C	4.612423	1.409357	4.965379
C	4.540806	2.606179	5.714851
H	4.365685	3.559515	5.194195
C	4.661513	2.600021	7.106849
H	4.590309	3.532335	7.683547
C	4.420336	1.435805	3.473613
H	3.368636	1.697692	3.231819
H	5.059702	2.207556	2.999261
H	4.638270	0.456681	3.010574
N	-0.751422	1.596830	1.592590
N	1.015458	-0.549203	2.297302
N	-5.782148	6.766467	-1.710134
H	-6.723435	6.460924	-1.452350
N	-5.272446	5.975987	-4.614113
H	-4.263095	6.059273	-4.438146
N	1.144996	3.368957	9.116488
H	1.847460	4.109398	9.051167
N	3.716483	2.275319	10.079425
H	4.051877	2.802219	10.897903
S	-5.771586	4.385895	-4.327425
S	5.054323	1.354630	9.544276
F	-4.816622	2.807240	0.717096
F	-6.500672	4.788184	-0.053310
F	-1.422094	4.670649	-2.028105
F	-3.041031	6.641870	-2.771888
F	-0.861762	0.084386	6.191880
F	-0.471687	1.006548	8.662711
F	1.775242	3.609205	4.400101
F	2.200119	4.545199	6.907216
O	-4.529434	3.635058	-4.036859
O	-6.935851	4.397977	-3.410470
O	4.933995	-0.053413	9.999988
O	6.228049	2.175834	9.913537

Conformation 21.
Multiplicity: 2
Charge: 0
E(B97-3c) = -9171.802089382092 Hartree
E(GFN1-xTB) = -378.642672725431 Hartree
E(GFN2-xTB) = -362.171421278556 Hartree
E(GFN-FF) = -35.167560773366 Hartree
E(M06/def2-TZVP) = -9172.841525071675 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -9169.259429012684 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -9169.498018702177 Hartree
E(PBEh-3c) = -9158.811838795891 Hartree
E(PM6) = -560.49513 Kcal/mol
E(PM7) = -670.89896 Kcal/mol
E(ωB97X-V/def2-TZVP) = -9174.400127570754 Hartree

Coordinates:

Cu	-0.021773	-1.880249	0.667461
C	-2.905758	-0.100785	-0.052799
C	-1.730496	0.624439	0.214424
C	-1.634641	2.067697	0.118363
H	-2.431541	2.731861	-0.234845
C	-0.357018	2.394856	0.491035
H	0.101414	3.387730	0.532285
C	0.327326	1.153320	0.796415
C	1.672923	1.082764	1.209727
C	2.378677	-0.117465	1.389259
C	3.752339	-0.186804	1.844541
H	4.365904	0.680312	2.111969
C	4.092656	-1.513748	1.884945
H	5.041616	-1.959475	2.204424
C	2.920879	-2.250928	1.447043
C	-4.121276	0.668288	-0.436527
C	-4.622206	0.645012	-1.748048
C	-5.721257	1.411665	-2.151736
C	-6.388927	2.278443	-1.255946
C	-5.891726	2.283517	0.073565
C	-4.788496	1.523769	0.463345
C	-7.824209	3.558652	-2.872869
H	-8.884329	3.889622	-2.852832
H	-7.774379	2.711799	-3.580066
C	-6.968975	4.735365	-3.394658
H	-7.268643	4.967285	-4.440553
H	-7.178054	5.640971	-2.791304
C	-3.696435	6.431302	-2.554881
C	-4.292715	7.701280	-2.548303
H	-5.333215	7.822422	-2.214609
C	-3.526369	8.807858	-2.934372
H	-3.982189	9.810382	-2.919568
C	-2.172791	8.669052	-3.308533
C	-1.602616	7.377469	-3.297928
H	-0.536011	7.261073	-3.543131
C	-2.354789	6.257793	-2.927979
H	-1.904414	5.255863	-2.887089
C	-1.335820	9.858708	-3.695179
H	-1.782754	10.808348	-3.341752
H	-1.239378	9.928230	-4.800018
H	-0.308307	9.759676	-3.291088
C	2.353967	2.387599	1.437363
C	1.945717	3.233215	2.483760
C	2.386344	4.558834	2.584452
C	3.226344	5.126344	1.597976
C	3.707713	4.249022	0.596572
C	3.278334	2.920613	0.516274
C	2.526283	7.429905	1.966773
H	2.576844	7.624734	3.057831
H	1.510693	7.015940	1.781892
C	2.647110	8.772972	1.258204
H	1.800212	9.404668	1.615574
H	3.588484	9.278627	1.562604
C	0.055542	7.668551	-0.351129
C	-0.686751	8.845741	-0.182635
H	-0.272659	9.817284	-0.491609
C	-1.974839	8.757351	0.360622
H	-2.570202	9.674096	0.491538
C	-2.537412	7.515183	0.726189
C	-1.761938	6.347932	0.541828
H	-2.184535	5.365350	0.803450
C	-0.472470	6.417417	0.007600
H	0.134144	5.516148	-0.159518
C	-3.933212	7.418529	1.276798

H	-3.932232	6.938040	2.277049
H	-4.569169	6.788299	0.619842
H	-4.406525	8.414274	1.372463
N	-0.522266	0.086436	0.607064
N	1.886622	-1.385160	1.160247
N	-7.469561	3.090491	-1.546562
H	-7.632920	3.771205	-0.799806
N	-5.530405	4.515643	-3.348615
H	-5.170729	3.632408	-3.728872
N	3.554959	6.474198	1.558671
H	3.961546	6.711943	0.646987
N	2.694577	8.679409	-0.203986
H	2.802415	9.576824	-0.688340
S	-4.628730	5.007463	-2.006917
S	1.659485	7.711484	-1.149979
F	-4.028342	-0.121745	-2.682775
F	-6.050588	1.386274	-3.472159
F	-4.360780	1.623861	1.728831
F	-6.486552	3.107517	0.961172
F	1.079498	2.784196	3.403516
F	1.962217	5.304235	3.629051
F	3.704704	2.169015	-0.508032
F	4.533006	4.748965	-0.341409
O	-3.654877	3.926792	-1.729694
O	-5.596076	5.484946	-0.981806
O	1.559352	8.466871	-2.423373
O	2.177990	6.329647	-1.133478
C	2.872901	-3.653706	1.341886
C	1.721474	-4.377894	0.975676
C	1.685005	-5.821259	0.848419
H	2.539109	-6.488072	1.005770
C	0.401837	-6.155482	0.502328
H	-0.015797	-7.153636	0.333881
C	-0.341625	-4.915310	0.407124
C	-1.708910	-4.844921	0.082698
C	-2.445787	-3.644199	0.016242
C	-3.859876	-3.573246	-0.294029
H	-4.511884	-4.427393	-0.497541
C	-4.197664	-2.245029	-0.298160
H	-5.180312	-1.797434	-0.480916
C	-2.984404	-1.505194	-0.027243
C	4.114964	-4.419269	1.640493
C	4.235699	-5.217811	2.795870
C	5.401400	-5.930217	3.075657
C	6.541665	-5.886314	2.230939
C	6.406743	-5.095205	1.068518
C	5.239298	-4.369172	0.800947
C	9.001075	-6.430510	2.132120
H	9.582230	-7.348434	2.363492
H	8.990194	-6.338094	1.030232
C	9.745057	-5.228144	2.750379
H	10.777116	-5.192355	2.335201
H	9.843398	-5.373064	3.845387
C	9.066700	-2.055166	4.531039
C	9.274438	-0.822508	3.890196
H	8.814038	-0.629643	2.910401
C	10.053526	0.147301	4.526948
H	10.216653	1.117708	4.032030
C	10.625665	-0.088692	5.798211
C	10.385658	-1.330782	6.418270
H	10.809919	-1.527851	7.415192
C	9.607013	-2.317717	5.795770
H	9.398619	-3.279610	6.285469
C	11.465362	0.970177	6.464351
H	12.386688	1.174738	5.879345
H	10.914996	1.930574	6.539356
H	11.771870	0.669790	7.484393
C	-2.420414	-6.098975	-0.288257
C	-3.505937	-6.600964	0.452425
C	-4.272195	-7.692323	0.018230
C	-3.994783	-8.347147	-1.204980
C	-2.869306	-7.869400	-1.920641
C	-2.111686	-6.784202	-1.480113
C	-6.162764	-9.506538	-1.576282
H	-6.470202	-10.479853	-2.013238
H	-6.437936	-9.538209	-0.506046
C	-6.929855	-8.364096	-2.257685
H	-6.616765	-7.397225	-1.810056
H	-8.021501	-8.464178	-2.060590
C	-5.637759	-5.833221	-4.218019
C	-5.867906	-4.535996	-3.739435
H	-6.897789	-4.217762	-3.522775
C	-4.773366	-3.681805	-3.540349
H	-4.935037	-2.661054	-3.163694
C	-3.455430	-4.111381	-3.799037
C	-3.262707	-5.419929	-4.299669
H	-2.241225	-5.777366	-4.496906
C	-4.341757	-6.279730	-4.521758
H	-4.182789	-7.300889	-4.894210
C	-2.274463	-3.217361	-3.528899
H	-1.562260	-3.715111	-2.839587
H	-1.717396	-2.999323	-4.464020
H	-2.581171	-2.257283	-3.074130
N	0.479694	-3.846118	0.699162
N	-1.934509	-2.374476	0.185718
N	7.645380	-6.629192	2.605759
H	7.575242	-6.927001	3.581826
N	9.096521	-3.942048	2.537772
H	8.699203	-3.774188	1.604777
N	-4.712793	-9.416826	-1.715835
H	-4.402883	-9.630261	-2.667627
N	-6.604085	-8.320485	-3.682032
H	-6.993334	-9.099187	-4.232545
S	8.066106	-3.300122	3.717939
S	-7.039712	-6.899906	-4.543300
F	3.210898	-5.304855	3.654616
F	5.491070	-6.657383	4.208789
F	5.218588	-3.606281	-0.300683
F	7.462051	-4.921526	0.222129
F	-3.847803	-6.019028	1.610583
F	-5.299670	-8.101159	0.794094
F	-1.101462	-6.355280	-2.256947
F	-2.574196	-8.460068	-3.101719
O	7.007579	-2.591757	2.964613
O	7.771987	-4.346456	4.726265
O	-8.235385	-6.269128	-3.936902
O	-7.030693	-7.329862	-5.956757

Conformation 29.
Multiplicity: 2
Charge: 0
E(B97-3c) = -9171.809104614103 Hartree
E(GFN1-xTB) = -378.648897551350 Hartree
E(GFN2-xTB) = -362.172770499308 Hartree
E(GFN-FF) = -35.184973048727 Hartree
E(M06/def2-TZVP) = -9172.850888596924 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -9169.266976840323 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -9169.504437265598 Hartree
E(PBEh-3c) = -9158.820500071699 Hartree
E(PM6) = -565.65965 Kcal/mol
E(PM7) = -678.72587 Kcal/mol
E(ωB97X-V/def2-TZVP) = -9174.407289092167 Hartree

Coordinates:

Cu	-0.702032	-0.611871	-1.622842
C	1.465364	2.077746	-1.448617
C	0.747292	1.730773	-0.287205
C	0.897217	2.399331	0.990755
H	1.573897	3.234501	1.196557
C	0.057473	1.768776	1.872089
H	-0.101198	2.010070	2.929371
C	-0.599122	0.708586	1.128935
C	-1.566260	-0.152058	1.684147
C	-2.282641	-1.112133	0.952132
C	-3.384049	-1.886592	1.488020
H	-3.763129	-1.807712	2.512667
C	-3.847180	-2.678724	0.469336
H	-4.694657	-3.373968	0.483605
C	-2.992027	-2.416532	-0.675000
C	2.409886	3.221540	-1.332598
C	3.805248	3.039227	-1.281597
C	4.676680	4.089146	-0.991246
C	4.213969	5.388114	-0.654452
C	2.816241	5.587567	-0.784806
C	1.951211	4.529394	-1.092884
C	4.729697	7.453422	0.614724
H	4.039487	8.112195	0.055297
H	5.645394	8.042142	0.822542
C	4.054669	7.058816	1.953333
H	3.321682	7.843665	2.234967
H	3.457813	6.132254	1.811718
C	5.107196	4.152973	3.302217
C	4.423413	3.874592	4.495751
H	4.480670	4.574176	5.339668
C	3.685572	2.689649	4.590379
H	3.144847	2.456647	5.520208
C	3.616174	1.778826	3.513154
C	4.315053	2.090353	2.325833
H	4.272546	1.400154	1.468641
C	5.072369	3.263940	2.217187
H	5.648941	3.486766	1.311184
C	2.842029	0.497779	3.645756
H	2.166775	0.513503	4.521497
H	3.532136	-0.363384	3.774695
H	2.234144	0.294431	2.743487
C	-1.799134	0.004714	3.147830
C	-2.850285	0.767620	3.677978
C	-2.910386	1.113864	5.036472
C	-1.885576	0.743630	5.937456
C	-0.865263	-0.087330	5.408750
C	-0.823733	-0.439037	4.061401
C	-2.520351	2.222680	7.858164

H	-2.319969	2.194396	8.950466
H	-3.610700	2.074283	7.733790
C	-2.153547	3.614464	7.308289
H	-2.324876	3.651401	6.214312
H	-2.823251	4.376175	7.761914
C	1.646018	4.744257	6.582220
C	2.669548	4.748064	7.542056
H	2.740137	3.928694	8.271885
C	3.611006	5.784547	7.519733
H	4.428412	5.786634	8.257326
C	3.556021	6.805104	6.545235
C	2.506560	6.772117	5.601349
H	2.453206	7.553542	4.828814
C	1.550054	5.750438	5.610018
H	0.747723	5.708198	4.859645
C	4.641815	7.843225	6.472154
H	4.323124	8.730977	5.892156
H	5.534831	7.405590	5.974444
H	4.956532	8.178808	7.480179
N	-0.165492	0.703773	-0.179375
N	-2.066118	-1.441579	-0.368576
N	5.122574	6.337831	-0.237754
H	6.017905	5.923136	0.049169
N	4.904744	6.868662	3.125087
H	5.366351	7.720813	3.470857
N	-1.799105	1.108714	7.268354
H	-0.855638	0.956521	7.638742
N	-0.776032	4.042026	7.549636
H	-0.473537	3.974813	8.530949
S	6.091294	5.641614	3.183716
S	0.461162	3.404423	6.564403
F	4.332681	1.809850	-1.450129
F	6.002456	3.843784	-0.885089
F	0.637106	4.788008	-1.126439
F	2.268840	6.801053	-0.541393
F	-3.814997	1.226821	2.868110
F	-3.942181	1.891292	5.447151
F	0.209965	-1.175965	3.623377
F	0.129211	-0.476786	6.234002
O	6.792494	5.907777	4.459399
O	6.873560	5.572725	1.920049
O	1.108908	2.242253	7.235249
O	-0.114043	3.273660	5.206317
C	-3.070076	-3.116849	-1.893540
C	-2.195972	-2.907350	-2.978998
C	-2.204100	-3.709811	-4.186232
H	-2.891995	-4.538224	-4.384654
C	-1.197019	-3.233461	-4.984993
H	-0.901727	-3.578069	-5.981678
C	-0.581800	-2.133863	-4.269398
C	0.462057	-1.347405	-4.792004
C	0.983590	-0.204082	-4.152868
C	1.978628	0.676116	-4.733009
H	2.446366	0.550888	-5.713524
C	2.211167	1.668482	-3.816577
H	2.888646	2.524653	-3.903108
C	1.399495	1.363910	-2.657808
C	-4.109683	-4.173154	-2.036523
C	-5.210560	-4.009003	-2.901565
C	-6.180101	-5.000047	-3.048389
C	-6.130613	-6.224129	-2.330961
C	-5.014326	-6.388189	-1.481635
C	-4.052568	-5.382316	-1.325256
C	-7.507753	-8.226607	-1.665233
H	-8.138815	-8.936488	-2.240946
H	-6.593760	-8.780455	-1.381025
C	-8.285858	-7.819563	-0.396542
H	-8.541472	-8.738555	0.177149
H	-9.245144	-7.342814	-0.683532
C	-8.963196	-4.882630	1.731271
C	-8.436967	-4.816132	3.031488
H	-7.358082	-4.953361	3.193198
C	-9.302174	-4.554695	4.097907
H	-8.896280	-4.495124	5.120012
C	-10.685557	-4.353244	3.888678
C	-11.176942	-4.409561	2.568990
H	-12.248321	-4.235248	2.383519
C	-10.325754	-4.670841	1.485661
H	-10.699371	-4.694128	0.452115
C	-11.606483	-4.098162	5.053479
H	-11.821486	-5.041610	5.599696
H	-11.152975	-3.399754	5.785029
H	-12.576153	-3.676751	4.725779
C	1.099953	-1.777597	-6.066267
C	1.064958	-1.010566	-7.244318
C	1.780728	-1.369597	-8.395821
C	2.588566	-2.530880	-8.429918
C	2.586875	-3.320558	-7.253417
C	1.869310	-2.957729	-6.114331
C	4.001692	-2.016258	-10.413108
H	4.467218	-2.617366	-11.222200
H	3.258934	-1.355375	-10.896838
C	5.068798	-1.154683	-9.722951
H	4.587737	-0.553236	-8.923072
H	5.503897	-0.427587	-10.445703
C	6.125336	-1.388159	-6.443976
C	5.912901	-0.226630	-5.689409
H	6.304978	0.732547	-6.056924
C	5.199716	-0.320563	-4.485258
H	5.024406	0.581888	-3.881212
C	4.688778	-1.554583	-4.033395
C	4.931895	-2.708017	-4.814854
H	4.527065	-3.677213	-4.487621
C	5.654704	-2.637520	-6.008993
H	5.829620	-3.535316	-6.617532
C	3.886591	-1.650035	-2.762489
H	2.892232	-2.097466	-2.964169
H	4.390577	-2.304775	-2.021123
H	3.729861	-0.657293	-2.301302
N	-1.202669	-1.954571	-3.051442
N	0.638096	0.238443	-2.893247
N	-7.146875	-7.134692	-2.547975
H	-7.936280	-6.699374	-3.031115
N	-7.581170	-6.889870	0.474347
H	-6.580758	-7.065020	0.630569
N	3.330703	-2.954526	-9.519884
H	3.934955	-3.737420	-9.256565
N	6.071507	-2.011569	-9.093388
H	6.697870	-2.492830	-9.754373
S	-7.859257	-5.224471	0.360898
S	7.110848	-1.283313	-7.937082
F	-5.339619	-2.875969	-3.604679
F	-7.238983	-4.793576	-3.858437
F	-3.050569	-5.606240	-0.463530
F	-4.900629	-7.495888	-0.694566
F	0.334151	0.112851	-7.287551
F	1.690647	-0.568331	-9.479721
F	1.971218	-3.733351	-5.021102
F	3.361515	-4.429616	-7.235818
O	-6.557270	-4.592824	0.670666
O	-8.614532	-4.940581	-0.882664
O	7.307484	0.151995	-8.246337
O	8.252403	-2.217070	-7.853423

Conformation 6.
Multiplicity: 2
Charge: 0
E(B97-3c) = -9171.783331992496 Hartree
E(GFN1-xTB) = -378.619697312255 Hartree
E(GFN2-xTB) = -362.139681941343 Hartree
E(GFN-FF) = -35.156845141281 Hartree
E(M06/def2-TZVP) = -9172.826593199343 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -9169.240990988814 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -9169.477401680941 Hartree
E(PBEh-3c) = -9158.794055561842 Hartree
E(PM6) = -559.99684 Kcal/mol
E(PM7) = -654.20383 Kcal/mol
E(ωB97X-V/def2-TZVP) = -9174.376911653364 Hartree

Coordinates:

Cu	1.158085	1.302710	0.488472
C	-0.204117	0.986277	-2.680991
C	0.377656	-0.154754	-2.095309
C	0.378358	-1.467913	-2.708029
H	-0.087215	-1.715780	-3.667206
C	1.045146	-2.303218	-1.850522
H	1.240999	-3.374215	-1.964159
C	1.445355	-1.501051	-0.712644
C	2.163357	-2.006208	0.387906
C	2.509285	-1.244726	1.520151
C	3.325816	-1.742566	2.610081
H	3.766982	-2.743420	2.659464
C	3.451480	-0.722121	3.515737
H	4.019244	-0.717826	4.453685
C	2.702932	0.397611	2.975990
C	-0.830376	0.855205	-4.025262
C	-0.075286	0.578240	-5.180579
C	-0.654099	0.476868	-6.453810
C	-2.041426	0.687143	-6.660633
C	-2.798920	0.963298	-5.489551
C	-2.215452	1.031973	-4.223325
C	-2.105797	0.984548	-9.142993
H	-1.038130	0.703310	-9.150737
H	-2.135980	2.095439	-9.290403
C	-2.775604	0.308113	-10.343141
H	-2.162450	0.507666	-11.247303
H	-2.803920	-0.791062	-10.199470
C	-6.802136	0.368722	-10.805023
C	-7.736042	1.340898	-10.426258
H	-7.601908	1.881072	-9.477789
C	-8.829344	1.590465	-11.269448
H	-9.570761	2.351568	-10.980613

C	-8.998854	0.882737	-12.476069
C	-8.039548	-0.098153	-12.820765
H	-8.159211	-0.666646	-13.756187
C	-6.944608	-0.364305	-11.994966
H	-6.203060	-1.132746	-12.256583
C	-10.173433	1.148037	-13.381117
H	-9.837502	1.421500	-14.402564
H	-10.811993	1.967195	-12.999766
H	-10.807332	0.243046	-13.485538
C	2.607855	-3.426702	0.348323
C	3.607473	-3.864275	-0.544815
C	4.068634	-5.181317	-0.536994
C	3.562999	-6.161153	0.359008
C	2.537958	-5.726455	1.233833
C	2.087207	-4.397535	1.223149
C	3.724146	-8.584770	1.079761
H	3.507981	-8.305476	2.127938
H	4.597782	-9.271354	1.107468
C	2.511810	-9.331086	0.500172
H	1.627130	-8.662340	0.549149
H	2.684103	-9.575452	-0.573533
C	-0.438365	-10.451465	1.718977
C	-1.311388	-9.673221	0.949620
H	-1.209652	-9.672475	-0.145087
C	-2.298892	-8.920252	1.601659
H	-2.987993	-8.301184	1.006352
C	-2.425704	-8.942546	3.004696
C	-1.533545	-9.749213	3.748816
H	-1.623408	-9.781928	4.846226
C	-0.542022	-10.505515	3.118155
H	0.150015	-11.138110	3.692336
C	-3.494540	-8.143717	3.703973
H	-3.077438	-7.576453	4.560616
H	-4.283003	-8.810602	4.113315
H	-3.983863	-7.425733	3.018636
N	1.021767	-0.199444	-0.876262
N	2.147388	0.063828	1.757792
N	-2.694564	0.600135	-7.870747
H	-3.711288	0.760205	-7.798284
N	-4.144876	0.738601	-10.647257
H	-4.270570	1.760477	-10.633068
N	4.119328	-7.418916	0.318432
H	4.755292	-7.563414	-0.465467
N	2.231462	-10.507039	1.318503
H	3.000861	-11.191589	1.358745
S	-5.406115	0.025221	-9.741313
S	0.836056	-11.409799	0.901627
F	1.249260	0.393211	-5.082467
F	0.156342	0.164625	-7.490835
F	-3.016500	1.306205	-3.175177
F	-4.122672	1.169464	-5.624888
F	4.151761	-3.001827	-1.412895
F	5.040228	-5.566468	-1.396592
F	1.120766	-4.062826	2.088971
F	1.952331	-6.594990	2.091687
O	-5.624496	0.770264	-8.468574
O	-5.121667	-1.422840	-9.723486
O	0.586640	-11.339457	-0.556527
O	1.014770	-12.701115	1.595753
C	2.579568	1.639540	3.625524
C	1.896276	2.747004	3.087348
C	1.736035	4.009033	3.781703
H	2.120974	4.230611	4.782349
C	1.025030	4.831169	2.947564
H	0.722730	5.869543	3.118847
C	0.747753	4.068081	1.747206
C	0.048850	4.579908	0.638560
C	-0.168932	3.863657	-0.555562
C	-0.828303	4.413385	-1.722206
H	-1.225747	5.428270	-1.809323
C	-0.857598	3.419745	-2.664476
H	-1.258960	3.470531	-3.681775
C	-0.257930	2.249100	-2.058078
C	3.208878	1.796857	4.965619
C	4.337561	2.618553	5.160100
C	4.916227	2.781677	6.417844
C	4.421944	2.122268	7.573990
C	3.284013	1.310146	7.372060
C	2.716728	1.137365	6.103116
C	5.005982	1.512936	9.948508
H	5.376048	2.104444	10.812764
H	3.947240	1.275806	10.162484
C	5.827410	0.208746	9.875386
H	5.727990	-0.333508	10.842542
H	6.902858	0.450850	9.753181
C	7.417087	-2.046115	7.458388
C	6.903262	-3.343267	7.297072
H	5.838118	-3.484597	7.063427
C	7.768667	-4.433250	7.424002
H	7.373420	-5.453460	7.297237
C	9.142588	-4.251459	7.704559
C	9.627836	-2.935844	7.841073
H	10.698142	-2.773048	8.042502
C	8.775615	-1.828462	7.718015
H	9.151855	-0.799345	7.806214
C	10.054443	-5.441050	7.857630
H	9.808140	-6.013947	8.776807
H	9.949634	-6.143841	7.005942
H	11.116600	-5.137693	7.925181
C	-0.572430	5.927140	0.760236
C	-0.209967	7.020855	-0.046303
C	-0.885493	8.249280	0.005685
C	-1.980281	8.452316	0.878458
C	-2.315463	7.359671	1.715704
C	-1.638504	6.142345	1.657175
C	-3.005386	10.469045	-0.162271
H	-3.526911	11.370153	0.223276
H	-2.068497	10.822076	-0.631586
C	-3.870023	9.776982	-1.225867
H	-3.325924	8.889593	-1.611795
H	-4.023770	10.453625	-2.096797
C	-5.249714	6.618679	-1.040173
C	-4.785267	5.749710	-2.036683
H	-4.859028	6.054049	-3.090436
C	-4.237596	4.514574	-1.659941
H	-3.872539	3.818381	-2.429732
C	-4.138071	4.144590	-0.302844
C	-4.630133	5.040132	0.675236
H	-4.550837	4.773821	1.739863
C	-5.195103	6.267574	0.318319
H	-5.566061	6.963364	1.083391
C	-3.503920	2.841933	0.105508
H	-2.607610	3.026952	0.733040
H	-4.202220	2.233344	0.716231
H	-3.191331	2.245759	-0.771421
N	1.287646	2.803730	1.851885
N	0.179570	2.548321	-0.784300
N	5.074688	2.354094	8.769782
H	5.984268	2.795029	8.613508
N	5.452690	-0.679342	8.783829
H	4.447674	-0.784673	8.596233
N	-2.702032	9.629570	0.992170
H	-3.520656	9.487265	1.589854
N	-5.120504	9.308577	-0.631544
H	-5.789379	10.055583	-0.396101
S	6.306406	-0.645648	7.322320
S	-6.028120	8.157119	-1.525861
F	4.875972	3.266674	4.118554
F	6.015937	3.550206	6.559350
F	1.664775	0.313768	5.997056
F	2.766977	0.574457	8.397668
F	0.809369	6.905832	-0.909977
F	-0.467255	9.245240	-0.805684
F	-2.061349	5.139675	2.446236
F	-3.365705	7.505436	2.555774
O	5.303639	-0.965150	6.282016
O	7.151917	0.571338	7.274961
O	-5.803579	8.335880	-2.979362
O	-7.381350	8.243490	-0.939683

Conformation 7.
Multiplicity: 2
Charge: 0
E(B97-3c) = -9171.803486829018 Hartree
E(GFN1-xTB) = -378.640401965703 Hartree
E(GFN2-xTB) = -362.163082368337 Hartree
E(GFN-FF) = -35.179162942748 Hartree
E(M06/def2-TZVP) = -9172.845246462613 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -9169.262780436151 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -9169.500659815854 Hartree
E(PBEh-3c) = -9158.815402316801 Hartree
E(PM6) = -559.75136 Kcal/mol
E(PM7) = -669.94150 Kcal/mol
E(ωB97X-V/def2-TZVP) = -9174.402940799999 Hartree

Coordinates:

Cu	-0.243331	0.800155	1.417999
C	1.546945	2.596664	-0.936514
C	1.672841	1.194213	-0.943973
C	2.485377	0.459077	-1.891966
H	3.068480	0.902856	-2.705289
C	2.379680	-0.865287	-1.558025
H	2.873322	-1.720274	-2.031010
C	1.489825	-0.940172	-0.416518
C	1.149578	-2.142218	0.235994
C	0.327809	-2.208927	1.378348
C	-0.019494	-3.444562	2.049489
H	0.334335	-4.438688	1.764431
C	-0.890232	-3.121626	3.055532
H	-1.411245	-3.797553	3.740320
C	-1.074148	-1.684686	2.999620
C	2.281684	3.379343	-1.968910

C	1.604288	4.101498	-2.971684
C	2.290099	4.863914	-3.919269
C	3.705460	4.932811	-3.952134
C	4.388877	4.183162	-2.964606
C	3.688083	3.450482	-1.995024
C	5.561253	6.404844	-4.831436
H	6.125135	6.025660	-3.962345
H	5.360785	7.487801	-4.659365
C	6.423570	6.219820	-6.087423
H	5.923983	6.670583	-6.973651
H	7.389124	6.747930	-5.959374
C	9.264426	3.979719	-6.707787
C	9.185133	3.086315	-7.788479
H	8.307247	2.432691	-7.893401
C	10.238258	3.040436	-8.705894
H	10.184549	2.341598	-9.555639
C	11.376145	3.867487	-8.559255
C	11.428871	4.742288	-7.456576
H	12.312341	5.385270	-7.319292
C	10.380749	4.804056	-6.525787
H	10.420737	5.472421	-5.653813
C	12.498893	3.802477	-9.562153
H	12.151191	4.107804	-10.571390
H	12.891089	2.768995	-9.658973
H	13.340697	4.462825	-9.279303
C	1.654504	-3.415941	-0.348219
C	2.550126	-4.268787	0.323769
C	3.024436	-5.464036	-0.235989
C	2.645558	-5.875978	-1.536635
C	1.733283	-5.016393	-2.201886
C	1.248423	-3.843092	-1.628797
C	3.761478	-8.141382	-1.642518
H	4.493358	-7.797455	-0.889841
H	4.345900	-8.636342	-2.446735
C	2.812334	-9.184663	-1.026627
H	2.146949	-9.608843	-1.805812
H	3.415199	-10.035871	-0.631401
C	-0.582432	-7.551727	-0.109053
C	-0.698744	-7.024649	-1.405935
H	-0.245479	-7.547316	-2.259990
C	-1.384276	-5.818641	-1.586649
H	-1.441375	-5.379392	-2.594304
C	-1.970784	-5.139509	-0.495146
C	-1.883037	-5.725034	0.783987
H	-2.373595	-5.235244	1.637197
C	-1.177783	-6.917920	0.988067
H	-1.098814	-7.370718	1.985957
C	-2.621282	-3.794395	-0.674061
H	-1.844269	-2.999535	-0.683384
H	-3.315166	-3.563562	0.156857
H	-3.168082	-3.722840	-1.635092
N	1.066574	0.323542	-0.062219
N	-0.311274	-1.145328	1.983551
N	4.315491	5.651494	-4.967518
H	3.628947	6.084559	-5.590098
N	6.683319	4.815176	-6.389160
H	5.836567	4.238705	-6.264105
N	3.092295	-6.989326	-2.211650
H	2.606249	-7.142600	-3.096492
N	1.951629	-8.599469	-0.015029
H	2.367042	-8.353249	0.888887
S	7.924723	4.031876	-5.513574
S	0.333264	-9.066557	0.149370
F	0.259147	4.089637	-3.025238
F	1.601275	5.555701	-4.854957
F	4.402505	2.789473	-1.076125
F	5.733590	4.156753	-2.939632
F	2.984428	-3.945328	1.550353
F	3.854070	-6.226625	0.518608
F	0.339468	-3.131347	-2.317345
F	1.280783	-5.409127	-3.418179
O	7.431646	2.654367	-5.308229
O	8.377963	4.896080	-4.396533
O	0.046139	-9.971171	-0.991631
O	0.130745	-9.488640	1.553153
C	-1.968909	-0.981314	3.830775
C	-2.215422	0.400339	3.729826
C	-3.128394	1.121529	4.593469
H	-3.702825	0.675016	5.411727
C	-3.095612	2.432420	4.195559
H	-3.635804	3.284364	4.621706
C	-2.151106	2.511461	3.099314
C	-1.791280	3.714990	2.465390
C	-0.792228	3.816302	1.476457
C	-0.368992	5.064362	0.874470
H	-0.765644	6.054701	1.114671
C	0.599369	4.752121	-0.042359
H	1.167837	5.437648	-0.679095
C	0.734772	3.310341	-0.034233
C	-2.733703	-1.770775	4.834343
C	-2.096290	-2.435903	5.902120
C	-2.797964	-3.277252	6.763337
C	-4.183406	-3.542245	6.605291
C	-4.826542	-2.827436	5.571455
C	-4.112958	-1.998364	4.696716
C	-5.974582	-5.206501	7.218497
H	-6.309815	-5.641640	8.183408
H	-6.780654	-4.523235	6.889730
C	-5.826668	-6.360195	6.205222
H	-6.779307	-6.935492	6.181681
H	-5.035772	-7.059650	6.545297
C	-3.787479	-7.485930	3.320441
C	-4.475634	-7.549761	2.098298
H	-5.134790	-6.725829	1.789597
C	-4.280506	-8.660485	1.271578
H	-4.804074	-8.710363	0.304306
C	-3.398608	-9.702860	1.634700
C	-2.738487	-9.615951	2.878297
H	-2.032200	-10.406853	3.169226
C	-2.922988	-8.514187	3.723536
H	-2.381572	-8.423246	4.675709
C	-3.119051	-10.842987	0.694002
H	-3.965505	-11.024110	0.003367
H	-2.223533	-10.620053	0.074398
H	-2.901862	-11.780230	1.242453
C	-2.548689	4.949184	2.808319
C	-1.951704	6.074074	3.405220
C	-2.645502	7.276692	3.602663
C	-3.994047	7.424551	3.199667
C	-4.602642	6.273424	2.640919
C	-3.906203	5.080001	2.452554
C	-4.162163	9.905486	3.169232
H	-4.956590	10.643467	3.407864
H	-3.352603	10.061870	3.905366
C	-3.615698	10.163779	1.757846
H	-2.823347	9.418354	1.534220
H	-3.130648	11.165146	1.709515
C	-3.834394	8.077719	-0.969239
C	-2.584957	7.673380	-1.458594
H	-1.839877	8.436744	-1.725083
C	-2.319102	6.302680	-1.591878
H	-1.344474	5.967931	-1.976432
C	-3.278088	5.334479	-1.229211
C	-4.533315	5.779148	-0.752964
H	-5.290397	5.038782	-0.454677
C	-4.824413	7.140740	-0.632312
H	-5.797589	7.478712	-0.250755
C	-2.977386	3.862395	-1.328842
H	-3.133757	3.364689	-0.350223
H	-3.656140	3.366522	-2.054020
H	-1.935020	3.677996	-1.648192
N	-1.630761	1.264106	2.828179
N	-0.096050	2.762667	0.921004
N	-4.771345	-4.437283	7.479141
H	-4.064388	-4.934816	8.025571
N	-5.488049	-5.936245	4.852894
H	-5.927949	-5.069695	4.518274
N	-4.745409	8.579228	3.343170
H	-5.641999	8.485053	2.858627
N	-4.679177	9.990846	0.770120
H	-5.390190	10.736183	0.773493
S	-3.891480	-5.996035	4.304546
S	-4.202699	9.828668	-0.871694
F	-0.779564	-2.278354	6.094504
F	-2.145062	-3.934468	7.744228
F	-4.785417	-1.434938	3.683737
F	-6.142926	-3.050465	5.295723
F	-0.671101	6.019800	3.798645
F	-1.990326	8.303446	4.186518
F	-4.543592	4.054953	1.860758
F	-5.886014	6.376052	2.226409
O	-3.778221	-4.838420	3.379347
O	-2.967613	-6.167823	5.453222
O	-2.943301	10.567001	-1.124131
O	-5.435864	10.129260	-1.627300

FIYMEI

Conformation 10.
Multiplicity: 4
Charge: 0
E(B97-3c) = -6436.941306932763 Hartree
E(M06/def2-TZVP) = -6437.190121005134 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -6434.685977871798 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -6435.145144706639 Hartree
E(PBEh-3c) = -6428.336065124559 Hartree
E(PM6) = -197.36108 Kcal/mol
E(PM7) = -368.28448 Kcal/mol
E(ωB97X-V/def2-TZVP) = -6440.934556400814 Hartree
E(GFN1-xTB) = -241.619561399440 Hartree
E(GFN2-xTB) = -236.798112939851 Hartree

E(GFN-FF) = -31.239323464338 Hartree

Coordinates:

Co	-0.519231	0.314856	0.002990
Si	-2.193774	2.477909	0.379173
O	-0.778459	2.365647	-0.698573
C	-1.578993	1.196086	1.583572
C	0.261373	4.119194	-1.998621
C	-0.650363	3.016267	-1.914222
C	0.446268	4.757513	-3.279981
C	-3.691956	2.022771	-0.666596
H	-3.763584	2.718650	-1.526450
H	-4.621984	2.136545	-0.075403
H	-3.651164	0.988579	-1.056361
C	-1.356350	2.588284	-3.030846
H	-2.034498	1.731331	-2.946773
C	0.992908	4.592404	-0.874096
H	0.838055	4.106222	0.095673
C	-0.288243	4.289103	-4.409179
H	-0.136984	4.781023	-5.382088
C	1.881380	5.650389	-1.000301
H	2.439842	6.004084	-0.120447
C	-2.430475	4.293962	0.817214
H	-1.597396	4.758822	1.371989
H	-3.353175	4.394956	1.425413
H	-2.582830	4.865006	-0.122170
C	-1.172747	3.230062	-4.282782
H	-1.730821	2.858592	-5.154743
C	1.368527	5.841516	-3.371377
H	1.512256	6.327315	-4.349066
C	2.073030	6.278772	-2.259423
H	2.782028	7.115483	-2.350510
Si	-0.486657	1.880688	2.942491
O	-1.630635	2.364863	4.158711
C	-1.578514	4.286934	5.604421
C	-1.315066	2.892334	5.375942
C	-1.264154	4.855431	6.892556
C	0.711396	0.626576	3.678319
H	1.302712	1.100818	4.486964
H	1.414844	0.312015	2.882263
H	0.224698	-0.279075	4.081636
C	-0.782483	2.107292	6.397849
H	-0.602610	1.039049	6.213264
C	-2.140583	5.117463	4.594407
H	-2.386555	4.662429	3.626308
C	-0.711426	4.022254	7.909289
H	-0.474263	4.462739	8.889644
C	-2.376810	6.463702	4.832792
H	-2.812371	7.094478	4.042801
C	0.580204	3.412988	2.654309
H	0.050199	4.283334	2.229337
H	1.462458	3.187413	2.025277
H	0.958798	3.717715	3.652793
C	-0.482761	2.677230	7.662188
H	-0.063182	2.034855	8.451435
C	-1.520045	6.243449	7.101017
H	-1.279194	6.679823	8.083103
C	-2.061200	7.031918	6.096192
H	-2.250980	8.100911	6.277254
Si	-2.946120	0.181373	2.372242
O	-3.356910	-1.006458	1.168562
C	-5.506647	-2.072307	0.884684
C	-4.153051	-2.098654	1.368427
C	-6.319657	-3.256672	1.028728
C	-2.549962	-0.766769	3.956916
H	-3.442347	-1.367607	4.226784
H	-2.361705	-0.049503	4.778759
H	-1.691935	-1.459619	3.881722
C	-3.649295	-3.251058	1.969078
H	-2.610497	-3.250134	2.326126
C	-6.063642	-0.919828	0.260738
H	-5.431457	-0.030900	0.146241
C	-5.768364	-4.414737	1.650687
H	-6.395798	-5.312707	1.756479
C	-7.370331	-0.925591	-0.206176
H	-7.784597	-0.027330	-0.688713
C	-4.499402	1.174247	2.787830
H	-4.923632	1.741383	1.937967
H	-4.224175	1.896153	3.583735
H	-5.294264	0.506057	3.177975
C	-4.460175	-4.405612	2.109963
H	-4.035518	-5.302021	2.586801
C	-7.658512	-3.225196	0.536361
H	-8.278365	-4.128904	0.645203
C	-8.175121	-2.088188	-0.067108
H	-9.210543	-2.084488	-0.440307
Si	1.705317	-2.153374	1.042330
O	2.095774	-3.561147	0.108714
C	1.080578	-0.982526	-0.273653
C	4.021032	-4.981917	-0.066373
C	2.748519	-4.681487	0.531034
C	4.706332	-6.190087	0.322478
C	0.354351	-2.623683	2.280683
H	0.777483	-2.947209	3.252514
H	-0.293684	-1.744873	2.453428
H	-0.283126	-3.437382	1.886483
C	2.200007	-5.543584	1.479597
H	1.221230	-5.307025	1.919756
C	4.617281	-4.113767	-1.023735
H	4.091597	-3.185928	-1.284738
C	4.114147	-7.047905	1.296349
H	4.643875	-7.966883	1.590632
C	5.844471	-4.425693	-1.592280
H	6.292456	-3.743157	-2.330236
C	3.289827	-1.725784	1.968245
H	4.103274	-1.470326	1.263150
H	3.164447	-0.903446	2.699281
H	3.598296	-2.630002	2.533720
C	2.889871	-6.724362	1.860746
H	2.435109	-7.389429	2.610989
C	5.964810	-6.478060	-0.284382
H	6.490185	-7.400880	0.008413
C	6.520877	-5.618528	-1.221303
H	7.493698	-5.858398	-1.677553
Si	0.092959	-1.983038	-1.493856
O	-1.058799	-0.670660	-1.896847
C	-2.069954	-0.667429	-4.105280
C	-2.173909	-0.878966	-2.690161
C	-3.242337	-0.898659	-4.917111
C	-1.011519	-3.347892	-0.825156
H	-1.695550	-3.691912	-1.627144
H	-0.399131	-4.210076	-0.497229
H	-1.633093	-2.999494	0.021523
C	-3.373108	-1.280135	-2.115191
H	-3.413172	-1.413178	-1.027177
C	-0.871533	-0.217501	-4.729132
H	0.000648	-0.004984	-4.100328
C	-4.455233	-1.319481	-4.296489
H	-5.340732	-1.494098	-4.926586
C	-0.816459	-0.019901	-6.100703
H	0.116383	0.334951	-6.564276
C	0.919932	-2.605979	-3.061173
H	1.474535	-1.825104	-3.611315
H	1.639537	-3.390472	-2.748432
H	0.177422	-3.058706	-3.748442
C	-4.518153	-1.499484	-2.923518
H	-5.455270	-1.813394	-2.440152
C	-3.145777	-0.687657	-6.324978
H	-4.038092	-0.868808	-6.944337
C	-1.960862	-0.262025	-6.907037
H	-1.906486	-0.105610	-7.995101
Si	2.418822	0.115095	-0.959096
O	3.812043	-0.887041	-1.192984
C	5.520218	-0.917869	-2.881475
C	5.056260	-0.501303	-1.585491
C	6.859888	-0.569097	-3.288198
C	2.833384	1.498691	0.252597
H	3.642592	2.152037	-0.129856
H	1.923937	2.122070	0.361558
H	3.119447	1.120684	1.252998
C	5.899298	0.223208	-0.743576
H	5.538881	0.510807	0.253820
C	4.700114	-1.677968	-3.762858
H	3.689442	-1.949204	-3.431598
C	7.686799	0.184793	-2.404553
H	8.706514	0.449054	-2.723359
C	5.175075	-2.085018	-5.001322
H	4.532022	-2.679179	-5.668135
C	2.108000	0.917181	-2.636646
H	2.140808	0.174286	-3.456474
H	1.139820	1.450593	-2.682425
H	2.910045	1.657913	-2.832364
C	7.210690	0.567832	-1.159934
H	7.854992	1.140457	-0.475332
C	7.312769	-1.002564	-4.569984
H	8.335664	-0.739392	-4.882327
C	6.492593	-1.743606	-5.408388
H	6.863159	-2.071827	-6.391535

Conformation 12.
Multiplicity: 4
Charge: 0
E(B97-3c) = -6436.930224371637 Hartree
E(M06/def2-TZVP) = -6437.178031120511 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -6434.675468905502 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -6435.134479386317 Hartree
E(PBEh-3c) = -6428.321613829956 Hartree
E(PM6) = -190.96799 Kcal/mol
E(PM7) = -316.01737 Kcal/mol
E(ωB97X-V/def2-TZVP) = -6440.924145447530 Hartree
E(GFN1-xTB) = -241.626368458921 Hartree
E(GFN2-xTB) = -236.791307689990 Hartree

E(GFN-FF) = -31.314329122815 Hartree

Coordinates:

Co	-0.808621	-0.180561	1.293930
Si	-3.261116	-2.851498	0.967150
O	-3.898316	-2.112642	-0.459024
C	-2.424696	-1.494634	1.936082
C	-5.920102	-2.835472	-1.587059
C	-4.486580	-2.723066	-1.530396
C	-6.523289	-3.454666	-2.744659
C	-2.208373	-4.310961	0.394054
H	-2.691499	-4.747688	-0.504660
H	-2.169106	-5.102484	1.166548
H	-1.172333	-4.037019	0.119636
C	-3.712150	-3.182404	-2.594761
H	-2.621596	-3.064317	-2.548685
C	-6.765473	-2.345870	-0.551413
H	-6.301270	-1.854231	0.311394
C	-5.694125	-3.924558	-3.804408
H	-6.164807	-4.392829	-4.682174
C	-8.144594	-2.471654	-0.633280
H	-8.780973	-2.084108	0.176865
C	-4.717131	-3.569045	1.943848
H	-5.410121	-2.779079	2.297854
H	-4.337626	-4.102821	2.840917
H	-5.305147	-4.290374	1.340222
C	-4.317827	-3.781590	-3.728118
H	-3.677197	-4.132456	-4.551361
C	-7.944598	-3.570290	-2.792929
H	-8.401051	-4.046015	-3.675077
C	-8.740365	-3.094266	-1.762100
H	-9.835178	-3.191397	-1.819837
Si	-3.517389	-0.028420	2.264961
O	-2.217635	1.201831	2.223638
C	-2.261370	3.278937	3.485643
C	-2.370842	2.576299	2.240230
C	-2.315202	4.722532	3.463655
C	-4.794891	0.476482	0.983740
H	-4.920245	1.578734	1.016664
H	-5.774539	0.033539	1.254889
H	-4.549403	0.155956	-0.042590
C	-2.590372	3.267247	1.055658
H	-2.683766	2.704270	0.118882
C	-2.101413	2.617149	4.735992
H	-2.094670	1.521228	4.753378
C	-2.509886	5.400595	2.225116
H	-2.545836	6.500389	2.221230
C	-1.970807	3.336291	5.915197
H	-1.848697	2.803536	6.870365
C	-4.427410	0.165696	3.908774
H	-3.820949	0.024308	4.818515
H	-5.252895	-0.576833	3.933167
H	-4.887240	1.174908	3.949749
C	-2.658209	4.683745	1.048754
H	-2.816927	5.206048	0.093674
C	-2.173915	5.429328	4.694593
H	-2.208339	6.529565	4.673075
C	-1.999829	4.755948	5.894084
H	-1.891838	5.319514	6.832960
Si	-1.373469	-2.066183	3.349292
O	0.098790	-1.096554	3.020026
C	2.045125	-1.400545	4.463201
C	0.944860	-0.605430	4.002391
C	2.906444	-0.839959	5.480658
C	-1.800628	-1.623265	5.132759
H	-1.007954	-2.024647	5.796698
H	-2.764077	-2.086448	5.426021
H	-1.862038	-0.534519	5.315277
C	0.724571	0.665186	4.513588
H	-0.123507	1.245476	4.132226
C	2.340586	-2.694405	3.946320
H	1.710768	-3.102506	3.148709
C	2.647137	0.468062	5.985594
H	3.315189	0.880688	6.756651
C	3.426633	-3.417487	4.417745
H	3.644220	-4.411197	3.998194
C	-0.880956	-3.883897	3.388730
H	-0.365774	-4.229349	2.474029
H	-1.786059	-4.510951	3.527757
H	-0.213647	-4.061024	4.255258
C	1.577561	1.207062	5.506078
H	1.375275	2.219389	5.887152
C	4.009031	-1.617047	5.944024
H	4.661599	-1.188229	6.720261
C	4.265222	-2.878258	5.428526
H	5.123735	-3.460476	5.795714
Si	1.777678	1.352545	0.485280
O	2.528418	2.203605	-0.817926
C	0.421678	0.271345	-0.254829
C	4.248505	3.881108	-0.862011
C	3.842559	2.509246	-0.996848
C	5.633611	4.219681	-1.087003
C	3.153443	0.474932	1.421582
H	3.890983	1.233730	1.753380
H	2.772728	-0.044567	2.320179
H	3.687722	-0.255953	0.786748
C	4.768693	1.534670	-1.363600
H	4.423951	0.499806	-1.484916
C	3.324262	4.910192	-0.523288
H	2.270407	4.636698	-0.374868
C	6.556926	3.193212	-1.444956
H	7.611049	3.460939	-1.614875
C	3.744624	6.226517	-0.395550
H	3.019719	7.013157	-0.136062
C	1.094970	2.724715	1.590267
H	0.320181	3.325024	1.077021
H	0.656759	2.333026	2.527924
H	1.923329	3.405865	1.874508
C	6.125798	1.882008	-1.582918
H	6.834866	1.089470	-1.867599
C	6.027928	5.583377	-0.944181
H	7.084529	5.844735	-1.113463
C	5.108586	6.565062	-0.604332
H	5.433909	7.611684	-0.501222
Si	1.090146	-1.360105	-0.900135
O	2.568288	-1.009531	-1.719755
C	4.441038	-2.344299	-2.417022
C	3.177381	-1.722219	-2.707899
C	5.138175	-3.032928	-3.477215
C	-0.078665	-2.303992	-2.033446
H	0.395769	-3.248401	-2.368061
H	-0.981047	-2.562451	-1.446474
H	-0.385472	-1.719894	-2.919526
C	2.637979	-1.799599	-3.990610
H	1.684541	-1.298001	-4.198169
C	5.026846	-2.295351	-1.119479
H	4.482825	-1.776512	-0.318940
C	4.553737	-3.093177	-4.775803
H	5.092076	-3.619382	-5.578803
C	6.255603	-2.889626	-0.869204
H	6.694540	-2.840050	0.138925
C	1.574915	-2.586174	0.450462
H	2.274618	-2.154151	1.187206
H	0.678154	-2.943279	0.994482
H	2.064407	-3.463611	-0.020662
C	3.328794	-2.489494	-5.018228
H	2.882662	-2.527790	-6.023719
C	6.398984	-3.632461	-3.182292
H	6.932690	-4.154801	-3.991963
C	6.949076	-3.562133	-1.910908
H	7.924311	-4.029650	-1.705717
Si	-0.494270	1.141443	-1.663649
O	0.086180	0.567819	-3.188300
C	0.101500	1.373130	-5.444011
C	0.759890	1.218678	-4.176622
C	0.814136	2.019634	-6.520201
C	-0.363116	3.017732	-1.760317
H	-0.989772	3.368946	-2.605868
H	-0.703200	3.524139	-0.838072
H	0.685031	3.315404	-1.951458
C	2.063798	1.670571	-4.000274
H	2.546060	1.517312	-3.028135
C	-1.224240	0.902701	-5.666527
H	-1.745672	0.401995	-4.838128
C	2.144657	2.483179	-6.299990
H	2.679958	2.976998	-7.125440
C	-1.835956	1.065452	-6.901667
H	-2.860651	0.696397	-7.061733
C	-2.297866	0.607030	-1.718330
H	-2.398942	-0.491414	-1.798548
H	-2.841091	0.906224	-0.802657
H	-2.811351	1.071331	-2.584995
C	2.750746	2.306143	-5.064699
H	3.780744	2.654820	-4.893525
C	0.151043	2.170085	-7.774580
H	0.691493	2.664433	-8.597353
C	-1.142744	1.706368	-7.963718
H	-1.635415	1.832365	-8.940122

Conformation 17.
Multiplicity: 4
Charge: 0
E(B97-3c) = -6436.925473889696 Hartree
E(M06/def2-TZVP) = -6437.177491592233 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -6434.672598511813 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -6435.127929786493 Hartree
E(PBEh-3c) = -6428.302559712051 Hartree
E(PM6) = -203.78526 Kcal/mol
E(PM7) = -376.19146 Kcal/mol
E(ωB97X-V/def2-TZVP) = -6440.921646399332 Hartree
E(GFN1-xTB) = -241.622693846788 Hartree
E(GFN2-xTB) = -236.788553791529 Hartree

E(GFN-FF) = -31.243048823054 Hartree

Coordinates:

Co	-0.135588	0.096099	-0.543206
Si	-1.391496	-1.527286	-2.397848
O	0.353128	-1.284840	-2.139171
C	-1.864548	0.154369	-1.731866
C	2.035966	-1.896527	-3.770519
C	1.361131	-2.151119	-2.533140
C	3.130538	-2.766374	-4.134568
C	-1.819927	-3.052294	-1.391830
H	-1.183370	-3.887796	-1.749954
H	-2.879782	-3.341419	-1.522359
H	-1.646029	-2.906711	-0.311403
C	1.723001	-3.214292	-1.719406
H	1.201641	-3.357297	-0.766211
C	1.671046	-0.833889	-4.647079
H	0.818859	-0.191847	-4.390016
C	3.489388	-3.843589	-3.271563
H	4.328271	-4.495912	-3.558615
C	2.362996	-0.624420	-5.831937
H	2.060102	0.196239	-6.500129
C	-1.689955	-1.943590	-4.204944
H	-1.469103	-1.095273	-4.875724
H	-2.756574	-2.225781	-4.330579
H	-1.075000	-2.820040	-4.496203
C	2.794225	-4.064678	-2.092459
H	3.070610	-4.893110	-1.423123
C	3.819182	-2.515318	-5.358432
H	4.655286	-3.176784	-5.634270
C	3.448644	-1.467934	-6.188541
H	3.991289	-1.292460	-7.129800
Si	-1.212190	1.586814	-2.724336
O	-1.161466	1.143943	-4.394872
C	-2.068498	2.262516	-6.314936
C	-0.959744	1.998002	-5.441219
C	-1.872362	3.143326	-7.440001
C	-2.158727	3.214753	-2.685467
H	-1.679069	3.900318	-3.414609
H	-2.131471	3.703087	-1.692771
H	-3.215001	3.088365	-2.994270
C	0.283428	2.577219	-5.688422
H	1.125946	2.351980	-5.019885
C	-3.349366	1.681000	-6.095723
H	-3.475686	1.002072	-5.241407
C	-0.587172	3.721236	-7.660873
H	-0.444834	4.391202	-8.522289
C	-4.408084	1.961475	-6.947743
H	-5.393653	1.505742	-6.767961
C	0.604261	1.941232	-2.234313
H	1.318485	1.303702	-2.788589
H	0.827712	1.838151	-1.139931
H	0.844809	3.004072	-2.445047
C	0.464152	3.438582	-6.802446
H	1.455611	3.883090	-6.978162
C	-2.983822	3.406713	-8.294596
H	-2.838093	4.078990	-9.154607
C	-4.223759	2.832638	-8.054811
H	-5.068989	3.048769	-8.725807
Si	-3.641107	0.290071	-1.212023
O	-3.919295	-1.133407	-0.273968
C	-5.978472	-2.389810	-0.161012
C	-5.049034	-1.456899	0.416785
C	-7.148248	-2.764650	0.597796
C	-4.130565	1.766463	-0.147334
H	-5.182133	1.633678	0.180096
H	-4.072259	2.713934	-0.716231
H	-3.503918	1.866384	0.757891
C	-5.283559	-0.935085	1.687715
H	-4.555012	-0.233218	2.116313
C	-5.780165	-2.958104	-1.451981
H	-4.886593	-2.667631	-2.020255
C	-7.354389	-2.205347	1.892698
H	-8.248952	-2.497889	2.463179
C	-6.692880	-3.857939	-1.983106
H	-6.523456	-4.288351	-2.981735
C	-4.829548	0.229832	-2.682276
H	-4.565342	-0.581875	-3.389246
H	-4.806213	1.185653	-3.245551
H	-5.871830	0.062421	-2.341148
C	-6.436957	-1.310620	2.421821
H	-6.595403	-0.883756	3.423809
C	-8.065114	-3.692205	0.019152
H	-8.957060	-3.978261	0.598344
C	-7.846205	-4.227896	-1.241025
H	-8.565462	-4.942644	-1.668938
Si	-0.348736	1.769700	2.136065
O	0.706318	2.448838	3.327008
C	0.549224	0.335098	1.339192
C	0.387464	4.547749	4.480913
C	0.361981	3.110695	4.468659
C	0.040417	5.236550	5.701437
C	-1.949806	1.349822	3.041267
H	-2.435327	2.289401	3.374975
H	-2.648892	0.811764	2.373518
H	-1.781264	0.724517	3.938548
C	0.051281	2.406219	5.630182
H	0.078356	1.307854	5.605146
C	0.761122	5.308588	3.336545
H	1.053781	4.773677	2.423378
C	-0.297912	4.480897	6.862278
H	-0.560801	5.015459	7.787720
C	0.773164	6.695471	3.378570
H	1.069721	7.269684	2.487740
C	-0.745674	3.150026	0.908351
H	0.159768	3.541056	0.406305
H	-1.440532	2.775560	0.130603
H	-1.242834	3.995018	1.426431
C	-0.281321	3.095062	6.824209
H	-0.526998	2.514038	7.726086
C	0.057932	6.663078	5.704389
H	-0.211282	7.188919	6.633853
C	0.411971	7.378753	4.570379
H	0.422105	8.479098	4.594036
Si	0.238818	-1.272162	2.265190
O	1.213641	-2.430779	1.422911
C	2.578364	-4.129453	2.473265
C	1.387273	-3.742830	1.766435
C	2.783123	-5.526783	2.774046
C	-1.553551	-1.867283	2.178524
H	-1.581893	-2.972398	2.264659
H	-2.139017	-1.466254	3.028174
H	-2.075171	-1.574192	1.245865
C	0.462617	-4.710627	1.374099
H	-0.430700	-4.400302	0.815314
C	3.558431	-3.177702	2.874342
H	3.397188	-2.117381	2.637181
C	1.810411	-6.485340	2.362408
H	1.977343	-7.547857	2.596573
C	4.698939	-3.582554	3.554349
H	5.448969	-2.833785	3.850582
C	0.769389	-1.278734	4.073964
H	1.749576	-0.785690	4.210189
H	0.015518	-0.761101	4.701194
H	0.846024	-2.324316	4.437790
C	0.677109	-6.080787	1.674951
H	-0.070460	-6.821603	1.352843
C	3.966580	-5.903063	3.476082
H	4.122852	-6.968419	3.708009
C	4.903496	-4.954479	3.859155
H	5.810888	-5.264389	4.399984
Si	2.394344	0.688912	1.085316
O	3.277865	0.084011	2.436842
C	5.554444	0.363879	3.160288
C	4.162029	0.705260	3.267900
C	6.488351	0.972961	4.077978
C	2.859370	2.507510	0.899937
H	3.965425	2.574094	0.843298
H	2.451808	2.946153	-0.032683
H	2.523016	3.111546	1.763295
C	3.731655	1.609117	4.235255
H	2.663586	1.852485	4.286042
C	6.037426	-0.553986	2.184061
H	5.316928	-1.020743	1.499004
C	6.011833	1.896480	5.054491
H	6.732159	2.357481	5.747492
C	7.387473	-0.867994	2.110821
H	7.743570	-1.583647	1.354319
C	3.127822	-0.270077	-0.360040
H	2.982283	-1.356532	-0.211732
H	2.693175	0.001715	-1.342171
H	4.216004	-0.060847	-0.412943
C	4.661679	2.204429	5.124766
H	4.293203	2.917096	5.878512
C	7.867947	0.625282	3.971591
H	8.580543	1.087921	4.672547
C	8.310575	-0.273605	3.012139
H	9.379335	-0.529192	2.948031

Conformation 18.
Multiplicity: 4
Charge: 0
E(B97-3c) = -6436.924701603536 Hartree
E(M06/def2-TZVP) = -6437.173838456212 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -6434.673377041958 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -6435.129349120991 Hartree
E(PBEh-3c) = -6428.303585225352 Hartree
E(PM6) = -187.22108 Kcal/mol
E(PM7) = -379.82743 Kcal/mol
E(ωB97X-V/def2-TZVP) = -6440.916929076919 Hartree
E(GFN1-xTB) = -241.623328003547 Hartree
E(GFN2-xTB) = -236.784160053833 Hartree

E(GFN-FF) = -31.238590539073 Hartree

Coordinates:

Co	0.050673	-0.300452	-0.397082
Si	-0.393277	-0.107640	-3.215536
O	0.599062	-1.230448	-2.239281
C	-0.678194	1.090682	-1.824365
C	2.657880	-2.261778	-2.989202
C	1.269119	-2.363361	-2.645672
C	3.371462	-3.477545	-3.301993
C	-1.846336	-1.100352	-3.879105
H	-1.471560	-2.077702	-4.248848
H	-2.277583	-0.573563	-4.754644
H	-2.654123	-1.262207	-3.145141
C	0.612920	-3.587847	-2.669669
H	-0.453848	-3.625509	-2.408933
C	3.353746	-1.018941	-3.033055
H	2.807545	-0.087435	-2.839350
C	2.675990	-4.722402	-3.290791
H	3.231680	-5.642318	-3.527573
C	4.701706	-0.971077	-3.360783
H	5.214552	0.002071	-3.405069
C	0.613762	0.374834	-4.728738
H	1.567223	0.871261	-4.481824
H	0.009209	1.086357	-5.329827
H	0.804141	-0.520635	-5.355794
C	1.322510	-4.772249	-2.994474
H	0.788605	-5.734268	-2.996816
C	4.759498	-3.389903	-3.619222
H	5.304328	-4.318436	-3.850119
C	5.412866	-2.167062	-3.646494
H	6.483068	-2.119781	-3.898342
Si	0.800027	2.132425	-1.366517
O	1.807366	2.395282	-2.750833
C	3.821174	3.706919	-2.898973
C	2.416767	3.541775	-3.156705
C	4.476553	4.906262	-3.361214
C	0.521292	3.802880	-0.566737
H	1.510761	4.256428	-0.353202
H	-0.023712	3.704574	0.390305
H	-0.031184	4.498795	-1.227479
C	1.710892	4.524214	-3.847496
H	0.640769	4.364654	-4.046760
C	4.580410	2.724715	-2.201203
H	4.071423	1.817918	-1.852782
C	3.719161	5.893342	-4.058166
H	4.225626	6.806660	-4.405449
C	5.933906	2.910030	-1.957038
H	6.499246	2.144273	-1.403580
C	1.993635	1.109535	-0.274382
H	2.659875	0.462598	-0.871719
H	1.592233	0.513389	0.587211
H	2.630617	1.841950	0.263809
C	2.366040	5.700317	-4.294155
H	1.786475	6.463380	-4.835758
C	5.870203	5.061059	-3.096233
H	6.372315	5.976016	-3.447924
C	6.584221	4.089167	-2.410293
H	7.657677	4.231264	-2.212985
Si	-2.318780	1.959013	-1.914982
O	-3.523001	0.708626	-1.887504
C	-5.695080	0.834638	-2.954040
C	-4.875197	0.846838	-1.771153
C	-7.128364	0.941411	-2.809813
C	-2.752226	3.123433	-0.504821
H	-3.852193	3.262406	-0.475967
H	-2.284503	4.118665	-0.623416
H	-2.425384	2.703632	0.463078
C	-5.474906	0.941035	-0.515029
H	-4.839134	0.934341	0.380242
C	-5.142245	0.710352	-4.259997
H	-4.055078	0.608472	-4.356845
C	-7.699400	1.044569	-1.507910
H	-8.792748	1.124059	-1.409797
C	-5.955887	0.705491	-5.383615
H	-5.509617	0.606758	-6.384890
C	-2.511131	2.901000	-3.545328
H	-2.290823	2.266802	-4.427838
H	-1.801916	3.755521	-3.564331
H	-3.537472	3.304369	-3.664200
C	-6.883874	1.038475	-0.387336
H	-7.324073	1.111400	0.618912
C	-7.933710	0.935647	-3.987598
H	-9.026030	1.020356	-3.875236
C	-7.364614	0.823105	-5.247058
H	-8.003837	0.819751	-6.143065
Si	-0.989467	-0.001910	2.455061
O	-0.230935	1.504651	2.008497
C	-0.320421	-1.344256	1.303981
C	-0.132862	3.601353	3.213498
C	0.483880	2.373675	2.786242
C	0.654855	4.545926	3.972175
C	-0.690503	-0.227819	4.297878
H	-1.103184	0.643191	4.846691
H	-1.213087	-1.141869	4.643517
H	0.385620	-0.306032	4.544906
C	1.808003	2.108784	3.124556
H	2.245906	1.161898	2.793890
C	-1.488015	3.919734	2.916426
H	-2.080382	3.197458	2.342202
C	2.009287	4.237801	4.292898
H	2.597218	4.964297	4.874315
C	-2.052063	5.116654	3.334201
H	-3.101346	5.342798	3.090961
C	-2.805546	0.379668	2.140208
H	-2.969440	0.543883	1.058908
H	-3.461483	-0.443169	2.477477
H	-3.091588	1.303249	2.681244
C	2.566660	3.038090	3.879342
H	3.609370	2.789940	4.130170
C	0.041925	5.766181	4.385398
H	0.644817	6.484658	4.962756
C	-1.279659	6.049873	4.074841
H	-1.732409	6.997994	4.402736
Si	-1.635602	-2.636752	0.971049
O	-2.551825	-2.700695	2.440390
C	-3.714987	-4.457867	3.587855
C	-3.722855	-3.359161	2.660682
C	-4.950397	-5.151619	3.858453
C	-1.088111	-4.423896	0.680432
H	-2.011678	-5.032788	0.585370
H	-0.507509	-4.539443	-0.255086
H	-0.497786	-4.851122	1.512608
C	-4.915663	-2.965163	2.053748
H	-4.914240	-2.110803	1.362216
C	-2.522396	-4.871255	4.246449
H	-1.595869	-4.318529	4.040142
C	-6.147528	-4.728479	3.208926
H	-7.086245	-5.263154	3.419528
C	-2.536961	-5.937878	5.133883
H	-1.608672	-6.246591	5.638398
C	-2.741701	-2.213927	-0.488636
H	-3.121248	-1.175536	-0.501085
H	-2.141787	-2.346279	-1.411625
H	-3.599371	-2.913461	-0.552623
C	-6.123991	-3.655577	2.330943
H	-7.050384	-3.325233	1.836605
C	-4.925832	-6.244505	4.775207
H	-5.867193	-6.777408	4.982319
C	-3.748333	-6.631730	5.398075
H	-3.750918	-7.477229	6.102905
Si	1.258343	-2.181559	1.885816
O	2.356546	-0.895099	2.264330
C	4.773784	-0.895819	2.239353
C	3.529153	-0.951215	2.958300
C	6.006884	-0.865264	2.990658
C	2.184900	-3.203472	0.600724
H	3.134768	-3.553145	1.055841
H	1.621046	-4.090851	0.258822
H	2.450105	-2.607049	-0.292878
C	3.527708	-0.974627	4.352141
H	2.563905	-0.997542	4.879689
C	4.831242	-0.864297	0.816997
H	3.891850	-0.888404	0.252880
C	5.963119	-0.896460	4.415394
H	6.908809	-0.872752	4.977918
C	6.047616	-0.808213	0.152125
H	6.065039	-0.800338	-0.947996
C	1.084526	-3.233586	3.446694
H	0.525773	-2.718120	4.249485
H	0.561375	-4.182877	3.219161
H	2.093787	-3.489576	3.829505
C	4.745997	-0.950775	5.077178
H	4.714207	-0.969269	6.177094
C	7.239013	-0.802212	2.273716
H	8.178413	-0.777371	2.847958
C	7.262683	-0.774016	0.887274
H	8.224170	-0.728987	0.353253

Conformation 21.
Multiplicity: 4
Charge: 0
E(B97-3c) = -6436.948845705947 Hartree
E(M06/def2-TZVP) = -6437.197132818631 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -6434.693598032518 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -6435.154494875779 Hartree
E(PBEh-3c) = -6428.340729661084 Hartree
E(PM6) = -179.27535 Kcal/mol
E(PM7) = -372.20256 Kcal/mol
E(ωB97X-V/def2-TZVP) = -6440.923738808847 Hartree
E(GFN1-xTB) = -241.632151007728 Hartree
E(GFN2-xTB) = -236.807479124003 Hartree

E(GFN-FF) = -31.334306081172 Hartree

Coordinates:

Co	-0.295620	-0.328207	-0.240347
Si	0.267711	1.803243	2.161075
O	1.301969	0.485178	2.623982
C	-1.058405	1.082967	1.055291
C	2.606073	0.217269	4.642393
C	2.500638	0.638989	3.273600
C	3.888267	0.313683	5.300306
C	1.334087	3.102094	1.323696
H	2.229405	3.323684	1.935863
H	0.758383	4.042209	1.229140
H	1.654165	2.777435	0.317059
C	3.623030	1.119461	2.602494
H	3.535694	1.389393	1.542989
C	1.493744	-0.302658	5.363222
H	0.526994	-0.370897	4.850494
C	5.009227	0.827474	4.584613
H	5.980849	0.898416	5.096928
C	1.629917	-0.719261	6.680154
H	0.759223	-1.119310	7.222178
C	-0.330582	2.600370	3.770692
H	-0.900347	1.917855	4.428500
H	-0.972539	3.476480	3.546591
H	0.547293	2.961268	4.346033
C	4.874093	1.219424	3.261562
H	5.737457	1.605356	2.698055
C	3.988044	-0.120054	6.656081
H	4.965488	-0.047383	7.158566
C	2.888542	-0.626866	7.332799
H	2.988995	-0.958157	8.377635
Si	-2.362456	0.169429	2.055523
O	-2.910785	-1.040437	0.943674
C	-4.970236	-2.265232	0.689222
C	-3.639782	-2.163000	1.220958
C	-5.708287	-3.488449	0.891880
C	-1.809671	-0.709163	3.627154
H	-2.641622	-1.357199	3.969588
H	-1.608688	0.022567	4.432673
H	-0.916823	-1.340567	3.488413
C	-3.083943	-3.233152	1.918412
H	-2.055069	-3.156045	2.289712
C	-5.553918	-1.219831	-0.078189
H	-4.965792	-0.310969	-0.249023
C	-5.107524	-4.559679	1.616709
H	-5.675819	-5.491441	1.760245
C	-6.819288	-1.363264	-0.627845
H	-7.247973	-0.552469	-1.235963
C	-3.863230	1.168533	2.639893
H	-4.391785	1.742753	1.857927
H	-3.540243	1.881145	3.427230
H	-4.594034	0.471145	3.099945
C	-3.818868	-4.430239	2.111861
H	-3.339805	-5.263057	2.648698
C	-7.011528	-3.595565	0.322485
H	-7.577338	-4.527772	0.478170
C	-7.555747	-2.560059	-0.423602
H	-8.559855	-2.665938	-0.862342
Si	-1.887025	2.401730	-0.000400
O	-0.773458	2.847450	-1.265423
C	-0.366878	4.948750	-2.398851
C	-1.049332	3.683576	-2.310840
C	-0.611056	5.798421	-3.541039
C	-3.472621	1.819242	-0.834462
H	-3.844273	2.597700	-1.528583
H	-4.269991	1.637170	-0.091288
H	-3.312138	0.882854	-1.398312
C	-1.927314	3.310240	-3.328580
H	-2.437022	2.343294	-3.257525
C	0.550558	5.384827	-1.402855
H	0.736100	4.727146	-0.547782
C	-1.521277	5.376793	-4.553721
H	-1.699466	6.033351	-5.418797
C	1.206073	6.602022	-1.515430
H	1.916536	6.916114	-0.735338
C	-2.280170	4.026485	0.886576
H	-1.376435	4.534608	1.275134
H	-2.973132	3.858859	1.735204
H	-2.771847	4.721661	0.174841
C	-2.163527	4.154406	-4.442618
H	-2.863971	3.821382	-5.224033
C	0.078311	7.045156	-3.622660
H	-0.109994	7.690294	-4.495117
C	0.967537	7.441721	-2.635341
H	1.491270	8.406122	-2.719217
Si	1.978673	-2.031759	-0.669620
O	0.454818	-2.392588	0.195996
C	1.362756	-0.560086	-1.618633
C	-0.007220	-4.595288	1.119050
C	0.411622	-3.234382	1.293953
C	-0.125853	-5.425672	2.296056
C	3.264111	-1.768533	0.661407
H	3.288581	-2.657574	1.323341
H	4.272861	-1.642723	0.225221
H	3.051661	-0.875477	1.271628
C	0.760548	-2.750243	2.548084
H	1.075675	-1.700961	2.633269
C	-0.327183	-5.153744	-0.151231
H	-0.208650	-4.531698	-1.046363
C	0.224158	-4.893071	3.571611
H	0.136667	-5.539601	4.458085
C	-0.783662	-6.458729	-0.263260
H	-1.031244	-6.868045	-1.254245
C	2.506306	-3.600531	-1.580024
H	1.810008	-3.957084	-2.358258
H	3.484180	-3.399718	-2.067153
H	2.664361	-4.418392	-0.847162
C	0.673463	-3.587122	3.689974
H	0.954906	-3.175894	4.671398
C	-0.598104	-6.763120	2.142044
H	-0.693452	-7.391550	3.041393
C	-0.928848	-7.268866	0.894032
H	-1.295936	-8.301671	0.796433
Si	0.133956	-0.889534	-2.968497
O	-1.393844	-0.796278	-2.032537
C	-3.477429	-1.377328	-3.160369
C	-2.442060	-1.690321	-2.221727
C	-4.551373	-2.329232	-3.331833
C	0.060615	-2.578177	-3.803515
H	-0.776987	-2.585382	-4.530528
H	1.002921	-2.763997	-4.358011
H	-0.105699	-3.412402	-3.097021
C	-2.469436	-2.877494	-1.509093
H	-1.679785	-3.066848	-0.775028
C	-3.497341	-0.172997	-3.918811
H	-2.671063	0.536028	-3.792739
C	-4.540711	-3.546116	-2.591218
H	-5.371246	-4.255541	-2.722142
C	-4.536472	0.104614	-4.794592
H	-4.535574	1.045987	-5.365241
C	0.006005	0.399646	-4.331033
H	-0.224670	1.406122	-3.934520
H	0.951489	0.461097	-4.906874
H	-0.794471	0.105668	-5.038476
C	-3.515932	-3.812328	-1.697927
H	-3.515207	-4.735606	-1.099422
C	-5.603256	-2.009436	-4.240122
H	-6.426132	-2.731212	-4.360225
C	-5.602867	-0.820215	-4.953657
H	-6.426625	-0.591665	-5.646734
Si	2.720888	0.603496	-2.148963
O	3.753302	0.858118	-0.781575
C	5.588824	2.331638	-0.290840
C	5.096508	1.051222	-0.729030
C	7.010038	2.513658	-0.115529
C	2.219936	2.341374	-2.654559
H	3.119242	2.990065	-2.646946
H	1.772353	2.395124	-3.664153
H	1.482493	2.749321	-1.939410
C	6.000686	0.029414	-1.022386
H	5.619176	-0.941187	-1.367074
C	4.713443	3.422456	-0.025862
H	3.637185	3.279402	-0.177358
C	7.897155	1.437478	-0.410953
H	8.979523	1.584854	-0.277024
C	5.206362	4.641255	0.416859
H	4.512470	5.472269	0.616204
C	3.778194	-0.165450	-3.520714
H	4.111265	-1.192602	-3.269396
H	3.183427	-0.231621	-4.455639
H	4.678446	0.444891	-3.737887
C	7.395982	0.227589	-0.865377
H	8.081668	-0.601027	-1.099465
C	7.480369	3.779258	0.346797
H	8.564148	3.915992	0.487238
C	6.601852	4.819583	0.611556
H	6.985904	5.787626	0.967753

Conformation 28.
Multiplicity: 4
Charge: 0
E(B97-3c) = -6436.938432602682 Hartree
E(M06/def2-TZVP) = -6437.188119901255 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -6434.683396410443 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -6435.143035577711 Hartree
E(PBEh-3c) = -6428.331893773785 Hartree
E(PM6) = -185.07246 Kcal/mol
E(PM7) = -366.33415 Kcal/mol
E(ωB97X-V/def2-TZVP) = -6440.922791451552 Hartree
E(GFN1-xTB) = -241.626167162324 Hartree
E(GFN2-xTB) = -236.802744885602 Hartree

E(GFN-FF) = -31.312004550772 Hartree

Coordinates:

Co	0.614867	-0.324012	0.771282
Si	1.554530	1.553354	2.747856
O	-0.106768	1.035352	2.352629
C	2.440714	0.639043	1.397542
C	-1.958803	2.476244	3.054221
C	-1.189669	1.273091	3.195150
C	-3.076413	2.681204	3.946835
C	1.809333	1.059468	4.551391
H	1.150318	1.684221	5.187766
H	2.859573	1.252663	4.851211
H	1.578877	0.000526	4.768228
C	-1.510714	0.347120	4.179758
H	-0.907534	-0.562080	4.272526
C	-1.681989	3.464375	2.070531
H	-0.840417	3.302386	1.391288
C	-3.373782	1.708192	4.944007
H	-4.232690	1.878617	5.610042
C	-2.474380	4.595919	1.949191
H	-2.256226	5.333021	1.162471
C	1.569211	3.432496	2.755026
H	1.316491	3.890732	1.783228
H	2.571387	3.792982	3.065850
H	0.831759	3.784247	3.504376
C	-2.603435	0.563699	5.056930
H	-2.834007	-0.192882	5.822083
C	-3.869048	3.855511	3.793209
H	-4.731284	3.993961	4.463032
C	-3.580147	4.793997	2.814742
H	-4.215438	5.683902	2.696204
Si	3.620944	1.610672	0.332226
O	5.071005	1.507664	1.285598
C	6.984290	2.368902	2.397200
C	6.269038	2.128914	1.171408
C	8.282850	2.991629	2.340694
C	3.924886	0.827612	-1.369598
H	3.908401	1.607032	-2.157672
H	3.141183	0.085763	-1.609161
H	4.903923	0.313211	-1.419613
C	6.829182	2.513873	-0.047131
H	6.284671	2.323097	-0.982723
C	6.433233	2.012717	3.660447
H	5.434250	1.553821	3.678270
C	8.824286	3.367643	1.075687
H	9.815449	3.844343	1.038555
C	7.137440	2.248262	4.833121
H	6.700844	1.970090	5.804523
C	3.356503	3.455959	0.033247
H	3.474625	4.061548	0.949870
H	2.366894	3.673187	-0.414217
H	4.129848	3.789357	-0.688259
C	8.105135	3.134143	-0.086247
H	8.524083	3.426295	-1.061364
C	8.978616	3.215000	3.565983
H	9.972805	3.687277	3.526811
C	8.422825	2.851124	4.783987
H	8.976647	3.033201	5.717645
Si	3.221180	-0.993323	1.824298
O	1.745879	-1.989280	1.614232
C	1.010444	-3.690898	3.171801
C	1.652856	-3.327448	1.944397
C	0.880840	-5.089241	3.500108
C	4.518600	-1.695870	0.652899
H	4.750525	-2.733825	0.966470
H	5.447195	-1.097678	0.745132
H	4.216345	-1.710225	-0.409051
C	2.171715	-4.305591	1.103105
H	2.659180	-4.006953	0.166209
C	0.510090	-2.716917	4.076934
H	0.624119	-1.659946	3.805583
C	1.407730	-6.067138	2.606859
H	1.304414	-7.132613	2.861925
C	-0.104599	-3.092070	5.261658
H	-0.483010	-2.324260	5.954161
C	3.870507	-1.393315	3.546935
H	3.139125	-1.273914	4.363970
H	4.746975	-0.747089	3.759496
H	4.221874	-2.445644	3.552157
C	2.045634	-5.678617	1.439067
H	2.454700	-6.435151	0.753062
C	0.235055	-5.441282	4.722759
H	0.130304	-6.508412	4.972791
C	-0.247071	-4.468095	5.585355
H	-0.739161	-4.759810	6.525271
Si	-0.044095	-2.277974	-1.764203
O	-0.833450	-2.193992	-3.304776
C	-0.560586	-0.727636	-0.853631
C	-1.705173	-3.873544	-4.788179
C	-0.638144	-2.995934	-4.387412
C	-1.541579	-4.678777	-5.974294
C	-0.597669	-3.940230	-1.061443
H	-0.317809	-4.721119	-1.799323
H	-0.103667	-4.190689	-0.103399
H	-1.693940	-3.999199	-0.920951
C	0.531680	-2.937864	-5.145112
H	1.330980	-2.247118	-4.845515
C	-2.923919	-3.952018	-4.057591
H	-3.038320	-3.319937	-3.168665
C	-0.325988	-4.598136	-6.714668
H	-0.208570	-5.216795	-7.617313
C	-3.950874	-4.786482	-4.474654
H	-4.890737	-4.828186	-3.903602
C	1.816892	-2.376359	-2.067992
H	2.175015	-1.544445	-2.703075
H	2.346832	-2.315056	-1.099100
H	2.091297	-3.331799	-2.558148
C	0.684194	-3.742937	-6.302852
H	1.618177	-3.673035	-6.881184
C	-2.617445	-5.527799	-6.371156
H	-2.494720	-6.140450	-7.278129
C	-3.796146	-5.581906	-5.641478
H	-4.615896	-6.240282	-5.967303
Si	-2.220895	-0.982911	-0.011551
O	-2.736232	0.588948	0.485722
C	-4.587007	2.104856	0.525252
C	-3.935142	0.928075	1.033495
C	-5.791794	2.570925	1.165341
C	-2.009029	-2.079599	1.521099
H	-2.980009	-2.507773	1.843968
H	-1.324930	-2.926597	1.325206
H	-1.603221	-1.504363	2.375723
C	-4.517678	0.214191	2.080381
H	-4.010232	-0.672504	2.479195
C	-4.076386	2.811940	-0.597840
H	-3.200581	2.398520	-1.111495
C	-6.344294	1.824957	2.247651
H	-7.268615	2.182381	2.726630
C	-4.699662	3.964031	-1.055087
H	-4.305220	4.483597	-1.941420
C	-3.628329	-1.640536	-1.074528
H	-3.646103	-1.114025	-2.047299
H	-3.549071	-2.731362	-1.246493
H	-4.587191	-1.450533	-0.549147
C	-5.723175	0.662960	2.677025
H	-6.149663	0.083270	3.509977
C	-6.394986	3.769066	0.681185
H	-7.307378	4.134740	1.178371
C	-5.858286	4.456870	-0.398038
H	-6.343795	5.376020	-0.760830
Si	-0.528845	0.765516	-1.992895
O	-2.095251	0.887731	-2.714486
C	-2.970729	1.005627	-4.945672
C	-2.445479	1.662117	-3.778981
C	-3.408654	1.808853	-6.061176
C	0.669526	0.742600	-3.446739
H	0.483695	1.661486	-4.040670
H	1.727743	0.757826	-3.124345
H	0.494138	-0.128169	-4.105517
C	-2.346125	3.053463	-3.749348
H	-1.954241	3.546261	-2.848810
C	-3.058416	-0.412459	-5.027542
H	-2.689441	-1.004202	-4.179687
C	-3.298463	3.229086	-5.989533
H	-3.634531	3.834570	-6.845140
C	-3.569354	-1.026459	-6.162575
H	-3.624782	-2.124356	-6.210889
C	-0.215220	2.333554	-0.994754
H	-1.081629	2.505878	-0.332111
H	0.681913	2.201300	-0.356402
H	-0.054605	3.219625	-1.640457
C	-2.772489	3.831348	-4.857214
H	-2.686402	4.927762	-4.804181
C	-3.933238	1.143266	-7.208718
H	-4.272149	1.753838	-8.060595
C	-4.014239	-0.240980	-7.259155
H	-4.419784	-0.735603	-8.155228

Conformation 31.
Multiplicity: 4
Charge: 0
E(B97-3c) = -6436.936324584732 Hartree
E(M06/def2-TZVP) = -6437.184131578867 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -6434.682408766176 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -6435.140825979824 Hartree
E(PBEh-3c) = -6428.328955652247 Hartree
E(PM6) = -195.38077 Kcal/mol
E(PM7) = -367.51279 Kcal/mol
E(ωB97X-V/def2-TZVP) = -6440.928890958168 Hartree
E(GFN1-xTB) = -241.620047850786 Hartree
E(GFN2-xTB) = -236.792528519718 Hartree

E(GFN-FF) = -31.239605509369 Hartree

Coordinates:

Co	-0.578519	-0.780766	0.502491
Si	-1.420593	-3.176036	-1.650673
O	-0.794595	-2.182519	-2.922356
C	-2.071473	-2.030546	-0.312073
C	-0.613515	-2.466504	-5.314127
C	-0.047008	-2.574481	-3.996251
C	0.194765	-2.832411	-6.453641
C	-0.025708	-4.343368	-1.151181
H	0.308633	-4.896958	-2.051040
H	-0.358172	-5.090696	-0.407693
H	0.844721	-3.802311	-0.739816
C	1.268404	-3.014108	-3.846004
H	1.699747	-3.071175	-2.838932
C	-1.941556	-2.003316	-5.530065
H	-2.537900	-1.709996	-4.659372
C	1.531542	-3.284851	-6.253774
H	2.139275	-3.558174	-7.129585
C	-2.464592	-1.909702	-6.811604
H	-3.492989	-1.546173	-6.959011
C	-2.745297	-4.273717	-2.438593
H	-3.591024	-3.701590	-2.864818
H	-3.154967	-4.985927	-1.692697
H	-2.291470	-4.862676	-3.262265
C	2.052690	-3.368771	-4.972922
H	3.087934	-3.707900	-4.816245
C	-0.376907	-2.724170	-7.756203
H	0.240867	-3.003743	-8.623965
C	-1.676822	-2.275597	-7.935038
H	-2.098773	-2.197803	-8.948644
Si	-3.683695	-1.229592	-0.823944
O	-3.796568	0.248337	0.080047
C	-5.827958	1.345123	0.794670
C	-4.724174	1.233793	-0.119848
C	-6.757931	2.437647	0.632955
C	-3.871762	-0.751813	-2.635010
H	-4.784310	-0.131586	-2.743572
H	-4.010036	-1.652742	-3.262760
H	-3.008883	-0.181723	-3.023091
C	-4.571913	2.165687	-1.145142
H	-3.718428	2.070600	-1.830491
C	-6.023738	0.421311	1.860308
H	-5.303663	-0.396108	1.982999
C	-6.568544	3.368625	-0.429384
H	-7.282223	4.198396	-0.545049
C	-7.089746	0.561255	2.737311
H	-7.222998	-0.159088	3.558693
C	-5.231226	-2.247785	-0.422439
H	-5.273392	-2.621788	0.618177
H	-5.283458	-3.124876	-1.099825
H	-6.139124	-1.632905	-0.593296
C	-5.497064	3.229363	-1.297911
H	-5.349226	3.951527	-2.114977
C	-7.841693	2.549854	1.554272
H	-8.549259	3.384854	1.431942
C	-8.007191	1.634917	2.583477
H	-8.849478	1.739960	3.284090
Si	-2.158875	-2.884278	1.343554
O	-0.480971	-2.512131	1.823002
C	1.008520	-3.745294	3.283757
C	0.053074	-2.693948	3.090589
C	1.614446	-3.887404	4.587054
C	-3.262269	-2.109038	2.655437
H	-2.990844	-2.517518	3.649565
H	-4.323317	-2.369101	2.472652
H	-3.173453	-1.007421	2.693731
C	-0.294139	-1.848190	4.136060
H	-1.007852	-1.034917	3.963150
C	1.389043	-4.637563	2.242682
H	0.921664	-4.526123	1.258431
C	1.239925	-2.998564	5.636969
H	1.712174	-3.114126	6.624368
C	2.331849	-5.630375	2.466941
H	2.615597	-6.309942	1.649129
C	-2.423831	-4.744530	1.500166
H	-1.850386	-5.367321	0.791066
H	-3.502851	-4.956468	1.347676
H	-2.163090	-5.063206	2.530799
C	0.302266	-2.003483	5.413633
H	0.021140	-1.306300	6.216431
C	2.579589	-4.919706	4.779563
H	3.042293	-5.025617	5.773141
C	2.933868	-5.772604	3.745046
H	3.682406	-6.561642	3.912747
Si	1.035565	1.110664	-1.908098
O	1.363410	2.805327	-1.703262
C	0.924324	0.482076	-0.138251
C	1.958891	4.527566	-3.270446
C	2.332691	3.591193	-2.246147
C	2.974632	5.389608	-3.826295
C	-0.601747	1.059090	-2.827580
H	-0.481101	1.485109	-3.844379
H	-0.925614	0.005061	-2.922356
H	-1.384211	1.634027	-2.297270
C	3.649892	3.527861	-1.798105
H	3.899386	2.798005	-1.017149
C	0.621020	4.627727	-3.747706
H	-0.140009	3.968595	-3.306952
C	4.314042	5.294428	-3.345732
H	5.082174	5.955281	-3.775889
C	0.288830	5.536628	-4.742414
H	-0.748947	5.603563	-5.103312
C	2.377231	0.399719	-3.013819
H	3.378271	0.451287	-2.547444
H	2.147878	-0.649332	-3.286002
H	2.400540	0.987878	-3.954272
C	4.636820	4.382565	-2.351429
H	5.670197	4.310008	-1.978738
C	2.594713	6.311334	-4.846955
H	3.368027	6.969461	-5.273797
C	1.284679	6.384532	-5.297438
H	1.013150	7.102546	-6.086498
Si	0.243784	1.869772	0.904715
O	-0.566462	0.806458	2.099816
C	-0.816791	1.610861	4.383312
C	-1.382556	1.309080	3.098555
C	-1.687965	2.145908	5.404606
C	-1.169220	2.882276	0.194037
H	-1.614242	3.513705	0.989324
H	-0.799917	3.541702	-0.614574
H	-1.970481	2.232375	-0.204011
C	-2.735693	1.508089	2.856546
H	-3.129779	1.245197	1.867996
C	0.553297	1.381472	4.694508
H	1.198007	0.936741	3.928881
C	-3.069347	2.349924	5.116313
H	-3.720792	2.760782	5.902726
C	1.058745	1.684723	5.950054
H	2.119873	1.494620	6.171450
C	1.413619	3.034078	1.803010
H	2.199351	2.518592	2.383223
H	1.903170	3.667070	1.034344
H	0.848914	3.693054	2.492825
C	-3.581306	2.029483	3.869083
H	-4.648645	2.173660	3.644945
C	-1.131342	2.448113	6.683186
H	-1.795340	2.861017	7.458642
C	0.211462	2.228215	6.952219
H	0.621641	2.468845	7.944793
Si	2.512279	-0.283214	0.462954
O	3.797251	0.744434	-0.089795
C	5.890249	1.374425	0.907967
C	5.137509	0.534936	0.014577
C	7.317874	1.189344	1.004785
C	2.799953	-2.014740	-0.222251
H	3.830562	-2.355058	0.001080
H	2.106886	-2.709137	0.292286
H	2.629999	-2.075838	-1.313440
C	5.795283	-0.417127	-0.764264
H	5.213157	-1.026470	-1.469399
C	5.265389	2.388479	1.687717
H	4.182307	2.533110	1.583913
C	7.950313	0.190493	0.207901
H	9.039631	0.054831	0.287604
C	6.010373	3.185950	2.544669
H	5.513136	3.968611	3.137622
C	2.765607	-0.424632	2.326569
H	2.941133	0.558553	2.802430
H	1.914255	-0.920074	2.830981
H	3.669799	-1.041244	2.508006
C	7.199761	-0.587429	-0.660484
H	7.692366	-1.348026	-1.285502
C	8.050403	2.025120	1.899589
H	9.139972	1.883480	1.976382
C	7.414330	2.999508	2.654719
H	7.998510	3.635647	3.337159

Conformation 32.
Multiplicity: 4
Charge: 0
E(B97-3c) = -6436.926851401521 Hartree
E(M06/def2-TZVP) = -6437.182742327684 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -6434.673450978057 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -6435.128781344029 Hartree
E(PBEh-3c) = -6428.311076536419 Hartree
E(PM6) = -200.04709 Kcal/mol
E(PM7) = -377.90056 Kcal/mol
E(ωB97X-V/def2-TZVP) = -6440.914021354466 Hartree
E(GFN1-xTB) = -241.619813306696 Hartree
E(GFN2-xTB) = -236.787893830313 Hartree

E(GFN-FF) = -31.249358800879 Hartree

Coordinates:

Co	0.091996	0.422823	0.157372
Si	-2.658438	0.512776	0.380856
O	-1.429894	1.562082	1.154541
C	-1.475070	-0.891578	0.034426
C	-1.590522	2.956142	3.119562
C	-1.625378	2.823424	1.694352
C	-1.753205	4.269594	3.692799
C	-3.347849	1.478251	-1.079165
H	-3.838573	2.402109	-0.712504
H	-4.101359	0.851999	-1.594586
H	-2.578475	1.762804	-1.821204
C	-1.842616	3.932647	0.884940
H	-1.885428	3.809327	-0.203631
C	-1.413709	1.839795	3.982183
H	-1.307843	0.845381	3.534727
C	-1.940023	5.391036	2.834109
H	-2.035637	6.392514	3.278714
C	-1.389167	2.002770	5.359755
H	-1.254917	1.126605	6.012362
C	-4.053525	0.310631	1.620246
H	-3.727661	-0.096104	2.594293
H	-4.817054	-0.368275	1.189099
H	-4.526838	1.297835	1.798591
C	-1.992214	5.220585	1.460654
H	-2.131589	6.088535	0.799805
C	-1.718309	4.399797	5.111782
H	-1.831257	5.404343	5.547293
C	-1.542193	3.294057	5.930091
H	-1.519343	3.415413	7.023649
Si	-1.369683	-2.226191	1.342081
O	-2.813032	-3.157694	1.136503
C	-4.168477	-4.332610	2.740803
C	-3.156451	-4.340765	1.719013
C	-4.585591	-5.586083	3.321855
C	0.151284	-3.318818	1.092982
H	-0.093624	-4.308000	0.664952
H	0.679372	-3.488083	2.052683
H	0.838045	-2.816169	0.387130
C	-2.613032	-5.550889	1.290049
H	-1.871182	-5.549824	0.480019
C	-4.781295	-3.125431	3.180079
H	-4.469849	-2.184684	2.710187
C	-3.993619	-6.800641	2.866579
H	-4.317962	-7.752765	3.313352
C	-5.757776	-3.141213	4.165393
H	-6.224572	-2.199357	4.491621
C	-1.361644	-1.741029	3.167323
H	-2.201698	-1.095838	3.482366
H	-0.409222	-1.255187	3.456134
H	-1.440911	-2.686136	3.745164
C	-3.031728	-6.776188	1.868439
H	-2.586166	-7.715547	1.507339
C	-5.590160	-5.563297	4.334909
H	-5.907106	-6.519190	4.780741
C	-6.162914	-4.370526	4.750857
H	-6.937872	-4.374766	5.532484
Si	-1.741167	-1.624370	-1.675563
O	-3.456087	-1.526080	-1.886238
C	-5.022214	-3.250064	-2.481781
C	-4.189084	-2.141423	-2.859122
C	-5.823306	-3.894627	-3.493099
C	-0.885179	-0.628399	-3.029688
H	-1.066427	-1.092660	-4.020228
H	0.205909	-0.666924	-2.835334
H	-1.209116	0.429043	-3.078383
C	-4.170107	-1.695237	-4.179022
H	-3.539764	-0.833697	-4.442580
C	-5.067881	-3.723823	-1.140415
H	-4.448143	-3.219188	-0.387555
C	-5.773055	-3.415119	-4.835766
H	-6.386147	-3.912484	-5.602906
C	-5.868642	-4.805556	-0.800857
H	-5.885392	-5.167229	0.238873
C	-1.258691	-3.421544	-1.937212
H	-1.791344	-4.098718	-1.244043
H	-0.166041	-3.566433	-1.833572
H	-1.541991	-3.706306	-2.971502
C	-4.964193	-2.337914	-5.164853
H	-4.932240	-1.968609	-6.201455
C	-6.637369	-5.000198	-3.105269
H	-7.250834	-5.496602	-3.873766
C	-6.658972	-5.447606	-1.791654
H	-7.291175	-6.305081	-1.513977
Si	3.112951	-0.856858	-0.606280
O	2.132312	-1.879189	-1.606221
C	2.083421	0.653496	-0.201197
C	2.726845	-4.089387	-2.421618
C	2.526227	-2.681818	-2.642775
C	3.074672	-4.926367	-3.547140
C	3.647643	-1.902327	0.879351
H	4.285514	-2.729291	0.506718
H	4.256198	-1.307567	1.590559
H	2.806535	-2.350954	1.439236
C	2.676067	-2.154135	-3.923406
H	2.514844	-1.080435	-4.074983
C	2.587927	-4.689451	-1.138018
H	2.315171	-4.053632	-0.289223
C	3.219626	-4.345149	-4.840176
H	3.485858	-4.992900	-5.689138
C	2.776879	-6.052433	-0.959982
H	2.659700	-6.494768	0.041033
C	4.725742	-0.499277	-1.520139
H	4.630905	0.171192	-2.392690
H	5.435546	-0.027982	-0.809680
H	5.175920	-1.452689	-1.865423
C	3.024339	-2.984959	-5.017746
H	3.134462	-2.534699	-6.015968
C	3.263101	-6.323197	-3.326056
H	3.526633	-6.957802	-4.186640
C	3.117679	-6.878055	-2.063678
H	3.265183	-7.958575	-1.915187
Si	2.018324	1.938278	-1.568691
O	3.262612	3.091310	-1.235618
C	5.144091	4.086891	-2.334373
C	3.731135	4.059099	-2.071520
C	5.676321	5.124411	-3.183735
C	0.327982	2.781566	-1.517519
H	0.178100	3.460463	-2.381841
H	-0.484649	2.023569	-1.578204
H	0.202297	3.350373	-0.579157
C	2.898412	5.020964	-2.643169
H	1.821375	4.998565	-2.427227
C	6.026908	3.114899	-1.785218
H	5.603214	2.328382	-1.147164
C	4.792975	6.092024	-3.746737
H	5.206445	6.880562	-4.393579
C	7.387211	3.158512	-2.055605
H	8.057933	2.398939	-1.626009
C	2.279926	1.449161	-3.369296
H	3.265552	0.996904	-3.581887
H	1.482198	0.767007	-3.719013
H	2.207776	2.382250	-3.965740
C	3.434100	6.033797	-3.479949
H	2.753521	6.781708	-3.914998
C	7.080186	5.139455	-3.436379
H	7.488649	5.932283	-4.082490
C	7.918407	4.180606	-2.886620
H	8.998837	4.209319	-3.094822
Si	2.548160	1.366265	1.471536
O	1.663752	2.852416	1.533370
C	1.549995	5.175722	2.081925
C	1.660124	3.806173	2.505581
C	1.420858	6.209203	3.079166
C	4.353531	1.828116	1.736322
H	4.472422	2.336536	2.715075
H	5.020322	0.942524	1.727515
H	4.671580	2.525885	0.937693
C	1.717456	3.506808	3.867168
H	1.784916	2.462698	4.194691
C	1.578777	5.536093	0.707022
H	1.758103	4.742779	-0.027107
C	1.470592	5.861540	4.460119
H	1.378630	6.656129	5.216107
C	1.433297	6.858960	0.315231
H	1.480449	7.123227	-0.752256
C	1.915119	0.253112	2.871602
H	0.879750	0.546273	3.135024
H	1.910346	-0.813574	2.581573
H	2.535217	0.352423	3.786007
C	1.631052	4.537360	4.836225
H	1.665042	4.265275	5.901719
C	1.257213	7.556852	2.640051
H	1.145334	8.346172	3.400147
C	1.251825	7.876228	1.290024
H	1.130004	8.923172	0.972316

Conformation 5.
Multiplicity: 4
Charge: 0
E(B97-3c) = -6436.931627283002 Hartree
E(M06/def2-TZVP) = -6437.186463712576 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -6434.677929941017 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -6435.133346286145 Hartree
E(PBEh-3c) = -6428.314276683425 Hartree
E(PM6) = -201.67427 Kcal/mol
E(PM7) = -375.26832 Kcal/mol
E(ωB97X-V/def2-TZVP) = -6440.919556404367 Hartree
E(GFN1-xTB) = -241.620647810536 Hartree
E(GFN2-xTB) = -236.792347449177 Hartree

E(GFN-FF) = -31.251117299767 Hartree

Coordinates:

Co	-0.457656	0.165330	-0.100154
Si	0.418786	2.753575	0.258132
O	0.090691	1.853944	-1.259339
C	0.596645	1.219179	1.322497
C	0.768432	2.385779	-3.515277
C	-0.225819	2.418731	-2.486413
C	0.443777	2.952310	-4.801626
C	-1.077316	3.863178	0.530152
H	-1.175671	4.557619	-0.327998
H	-0.922438	4.453961	1.452562
H	-2.025969	3.303578	0.634037
C	-1.469516	2.993921	-2.719229
H	-2.218389	3.009254	-1.918793
C	2.053255	1.809472	-3.313770
H	2.290137	1.389130	-2.329486
C	-0.844705	3.521495	-5.012715
H	-1.090408	3.929879	-6.004029
C	2.986272	1.780656	-4.340177
H	3.974901	1.328636	-4.168227
C	1.884602	3.873610	-0.081886
H	2.788981	3.335170	-0.416690
H	2.123826	4.431683	0.845867
H	1.603958	4.604735	-0.867364
C	-1.778292	3.542314	-3.989948
H	-2.779329	3.964101	-4.161323
C	1.428556	2.907649	-5.831025
H	1.175826	3.331528	-6.814937
C	2.671614	2.334260	-5.609894
H	3.417655	2.306010	-6.418471
Si	2.342662	0.547072	1.473606
O	3.148701	1.668759	2.517145
C	5.378830	2.492812	2.835419
C	4.343077	1.548662	3.158531
C	6.624139	2.441600	3.562200
C	2.447301	-1.181501	2.203086
H	3.511002	-1.462617	2.340126
H	2.002527	-1.905698	1.491319
H	1.933747	-1.289761	3.175724
C	4.557807	0.598635	4.156669
H	3.754200	-0.104466	4.412403
C	5.197981	3.488745	1.834881
H	4.241734	3.518249	1.298450
C	6.808556	1.448443	4.568094
H	7.762508	1.413188	5.115720
C	6.198815	4.409290	1.558810
H	6.041492	5.177313	0.786363
C	3.400853	0.473394	-0.086675
H	3.518814	1.443805	-0.602597
H	3.014369	-0.271798	-0.809002
H	4.413519	0.140475	0.222816
C	5.792729	0.549379	4.852547
H	5.932670	-0.211702	5.635288
C	7.631252	3.402767	3.249878
H	8.581208	3.366742	3.805986
C	7.425902	4.366627	2.273428
H	8.214388	5.101490	2.050256
Si	-0.161615	1.549793	3.006751
O	0.172860	3.228724	3.254297
C	1.241811	4.551818	4.945671
C	0.052040	3.955919	4.401736
C	1.131707	5.361057	6.134690
C	-2.032553	1.269267	3.046148
H	-2.423886	1.418945	4.072604
H	-2.253600	0.222914	2.754154
H	-2.587289	1.943019	2.364974
C	-1.181223	4.162904	5.017124
H	-2.084013	3.719298	4.574042
C	2.517101	4.359997	4.342524
H	2.582066	3.722829	3.450212
C	-0.145994	5.543934	6.742344
H	-0.220777	6.160103	7.651407
C	3.650891	4.948086	4.886465
H	4.630351	4.787393	4.411555
C	0.556491	0.678946	4.514282
H	1.647616	0.841876	4.595218
H	0.342084	-0.407581	4.528314
H	0.080526	1.129416	5.410143
C	-1.273662	4.955456	6.191263
H	-2.258687	5.103423	6.659936
C	2.318546	5.949326	6.663928
H	2.238560	6.568140	7.571630
C	3.549157	5.749468	6.054802
H	4.454041	6.210870	6.479312
Si	-0.801898	-3.065308	0.641127
O	0.858843	-3.492207	0.387022
C	-1.242946	-1.666547	-0.517211
C	2.015712	-5.416466	1.286197
C	1.384182	-4.736710	0.187967
C	2.581587	-6.725551	1.057943
C	-1.779129	-4.657950	0.379482
H	-1.424627	-5.434620	1.088009
H	-2.862251	-4.502309	0.551632
H	-1.652692	-5.055590	-0.645969
C	1.348850	-5.330776	-1.071591
H	0.880412	-4.786161	-1.901922
C	2.106452	-4.840761	2.585741
H	1.699923	-3.833892	2.743149
C	2.511820	-7.305387	-0.242628
H	2.944992	-8.304013	-0.405063
C	2.718381	-5.525164	3.626262
H	2.784567	-5.063020	4.622962
C	-0.912628	-2.545149	2.451103
H	-0.360386	-1.600539	2.616837
H	-1.962676	-2.391930	2.764742
H	-0.475430	-3.326250	3.104523
C	1.911206	-6.615051	-1.283581
H	1.864571	-7.060177	-2.289137
C	3.199682	-7.399724	2.152788
H	3.628860	-8.398804	1.978048
C	3.266337	-6.817343	3.409584
H	3.748901	-7.353566	4.240853
Si	-3.043901	-1.181528	-0.400090
O	-3.882799	-1.886825	-1.732070
C	-5.793719	-3.310400	-1.988520
C	-5.233954	-1.991838	-1.877176
C	-7.216740	-3.449325	-2.179337
C	-3.152855	0.705071	-0.527305
H	-4.171007	1.076156	-0.289078
H	-2.478332	1.194317	0.215084
H	-2.866127	1.041542	-1.540224
C	-6.062807	-0.872868	-1.947238
H	-5.620840	0.130592	-1.872872
C	-4.982546	-4.477573	-1.908303
H	-3.901184	-4.353445	-1.763376
C	-8.032197	-2.281380	-2.249172
H	-9.116967	-2.395919	-2.395281
C	-5.547063	-5.740929	-2.012680
H	-4.908473	-6.634967	-1.947861
C	-4.035010	-1.689040	1.123495
H	-4.009621	-2.776839	1.326130
H	-3.702566	-1.149044	2.031123
H	-5.093207	-1.409871	0.938732
C	-7.461584	-1.023430	-2.133072
H	-8.092767	-0.123300	-2.188383
C	-7.760313	-4.763888	-2.285693
H	-8.846224	-4.872860	-2.433429
C	-6.947164	-5.884838	-2.204340
H	-7.386554	-6.890534	-2.288034
Si	-0.623794	-1.912799	-2.270896
O	-1.258422	-0.523551	-3.095005
C	-2.362808	0.288882	-5.055189
C	-1.186291	-0.248448	-4.427327
C	-2.293805	0.704241	-6.434251
C	-1.306343	-3.387708	-3.222664
H	-0.933122	-3.358294	-4.266944
H	-1.014539	-4.360463	-2.781003
H	-2.411148	-3.323997	-3.240183
C	-0.023703	-0.427838	-5.177424
H	0.881997	-0.815515	-4.695963
C	-3.590785	0.417692	-4.350373
H	-3.637753	0.025162	-3.328115
C	-1.084641	0.513404	-7.164097
H	-1.041604	0.824058	-8.219160
C	-4.703609	0.981530	-4.957489
H	-5.652258	1.055267	-4.404217
C	1.264069	-1.851345	-2.348143
H	1.600787	-0.798202	-2.415915
H	1.700080	-2.311111	-1.441060
H	1.652982	-2.389498	-3.235937
C	0.016921	-0.055350	-6.544398
H	0.953553	-0.198888	-7.103495
C	-3.453385	1.291397	-7.022760
H	-3.399767	1.620273	-8.072674
C	-4.628852	1.438692	-6.300641
H	-5.513592	1.890405	-6.775044

Conformation 6.
Multiplicity: 4
Charge: 0
E(B97-3c) = -6436.929409885716 Hartree
E(M06/def2-TZVP) = -6437.181727031591 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -6434.676341929215 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -6435.134406632709 Hartree
E(PBEh-3c) = -6428.318436275017 Hartree
E(PM6) = -198.38159 Kcal/mol
E(PM7) = -371.42271 Kcal/mol
E(ωB97X-V/def2-TZVP) = -6440.922456065126 Hartree
E(GFN1-xTB) = -241.619865868035 Hartree
E(GFN2-xTB) = -236.789997096553 Hartree

E(GFN-FF) = -31.252154692759 Hartree

Coordinates:

Co	1.015841	-0.037062	-0.287927
Si	-1.962202	-0.040221	1.046870
O	-2.289842	-1.199636	-0.219832
C	-0.553523	1.046087	0.416418
C	-4.483474	-1.927808	-0.936063
C	-3.299149	-2.123139	-0.142914
C	-5.547339	-2.901105	-0.860588
C	-1.572195	-1.047009	2.597473
H	-2.447582	-1.679811	2.844471
H	-1.390835	-0.362907	3.448409
H	-0.695700	-1.710995	2.473215
C	-3.186033	-3.264643	0.650932
H	-2.269527	-3.425479	1.230958
C	-4.630894	-0.810815	-1.803607
H	-3.810866	-0.088059	-1.859356
C	-5.395018	-4.046349	-0.026836
H	-6.204841	-4.790266	0.014842
C	-5.777326	-0.642658	-2.566110
H	-5.868128	0.227391	-3.234029
C	-3.580516	0.860829	1.389814
H	-4.061623	1.248369	0.473028
H	-3.379581	1.703403	2.079696
H	-4.297554	0.167870	1.874963
C	-4.231021	-4.221552	0.703611
H	-4.104390	-5.113131	1.336188
C	-6.716346	-2.691899	-1.652055
H	-7.528044	-3.433294	-1.591607
C	-6.831665	-1.590844	-2.487928
H	-7.738780	-1.451980	-3.095482
Si	-1.087216	2.393025	-0.773172
O	-1.572779	3.732794	0.216316
C	-3.254328	5.427246	-0.081903
C	-1.885939	4.995529	-0.186044
C	-3.589324	6.781008	-0.453516
C	0.353878	2.941977	-1.860270
H	0.057355	3.780239	-2.521896
H	0.680064	2.099822	-2.503722
H	1.216549	3.261151	-1.247813
C	-0.907298	5.886957	-0.626294
H	0.138192	5.553412	-0.677526
C	-4.281731	4.559248	0.384991
H	-4.009301	3.538769	0.682929
C	-2.561175	7.659238	-0.905799
H	-2.824759	8.690889	-1.184267
C	-5.594993	4.998507	0.473320
H	-6.378427	4.317242	0.838338
C	-2.565523	2.165726	-1.917839
H	-3.505832	1.971060	-1.371004
H	-2.417519	1.372917	-2.673426
H	-2.695068	3.129414	-2.454113
C	-1.250283	7.215896	-0.985069
H	-0.457248	7.899915	-1.323886
C	-4.950546	7.195753	-0.351595
H	-5.207066	8.227400	-0.638972
C	-5.933068	6.326366	0.098550
H	-6.977948	6.665805	0.168327
Si	0.315291	1.816326	1.915877
O	-0.957191	2.069203	3.052839
C	-1.405873	3.934016	4.499475
C	-0.864541	2.618584	4.298221
C	-1.363930	4.509346	5.821165
C	1.556875	0.617443	2.689168
H	2.018674	1.086121	3.582850
H	2.393372	0.378537	2.001690
H	1.094294	-0.333713	3.006313
C	-0.314339	1.914262	5.367472
H	0.079724	0.902347	5.197130
C	-1.982424	4.671892	3.427653
H	-2.001253	4.212332	2.430749
C	-0.787174	3.761958	6.890746
H	-0.759493	4.206092	7.897454
C	-2.503502	5.939765	3.643870
H	-2.948730	6.496435	2.804975
C	1.233238	3.440053	1.690164
H	0.596419	4.244109	1.281260
H	2.123205	3.306445	1.044189
H	1.594706	3.757063	2.690358
C	-0.276946	2.492833	6.663083
H	0.160524	1.916550	7.492760
C	-1.908145	5.815401	6.004542
H	-1.880391	6.260643	7.011805
C	-2.465192	6.514863	4.942768
H	-2.879417	7.522117	5.106103
Si	3.131435	-0.324418	-2.117740
O	2.959939	0.768499	-0.718535
C	1.639432	-1.366221	-1.778880
C	4.815486	1.397228	0.720233
C	3.887171	1.720007	-0.323766
C	5.743776	2.418587	1.146023
C	3.111037	0.803780	-3.627562
H	3.819653	1.638685	-3.450368
H	3.458569	0.258176	-4.526461
H	2.115050	1.236289	-3.844172
C	3.909208	2.968392	-0.937239
H	3.194904	3.182338	-1.742306
C	4.860555	0.114696	1.337775
H	4.158916	-0.660442	1.002580
C	5.724773	3.695463	0.512098
H	6.436543	4.464732	0.848213
C	5.779042	-0.153904	2.342645
H	5.804822	-1.154203	2.799759
C	4.858400	-1.057710	-2.020349
H	5.023377	-1.633241	-1.092562
H	5.025596	-1.727502	-2.888809
H	5.613841	-0.246540	-2.060868
C	4.832244	3.959344	-0.514373
H	4.827245	4.943067	-1.007268
C	6.666241	2.107512	2.188676
H	7.371443	2.887678	2.515602
C	6.685618	0.850373	2.774004
H	7.406481	0.626795	3.574978
Si	1.860168	-2.904536	-0.726978
O	2.728182	-2.253476	0.662094
C	4.244606	-3.538394	2.059849
C	2.963955	-2.922450	1.833720
C	4.492155	-4.177378	3.332483
C	2.942374	-4.278221	-1.428914
H	3.271769	-4.956816	-0.615957
H	2.356909	-4.870298	-2.159173
H	3.844508	-3.886191	-1.937409
C	1.992394	-2.970491	2.830748
H	1.020538	-2.500409	2.637291
C	5.278359	-3.539639	1.081048
H	5.083405	-3.056648	0.117002
C	3.471212	-4.193849	4.326455
H	3.673443	-4.683183	5.291215
C	6.504707	-4.136879	1.332435
H	7.289572	-4.127333	0.561284
C	0.271973	-3.606864	-0.015391
H	-0.422780	-2.788217	0.253442
H	-0.241875	-4.234960	-0.765671
H	0.480054	-4.218592	0.884966
C	2.243785	-3.603204	4.073221
H	1.452175	-3.615434	4.837736
C	5.765183	-4.781765	3.556670
H	5.950250	-5.270044	4.526384
C	6.751401	-4.764255	2.582408
H	7.725800	-5.238224	2.776053
Si	0.605197	-1.777045	-3.282399
O	0.174744	-3.427543	-3.019939
C	-1.521281	-4.730036	-4.131476
C	-0.140646	-4.385812	-3.935846
C	-1.845373	-5.762677	-5.087253
C	1.484760	-1.746011	-4.957140
H	0.894817	-2.358816	-5.669794
H	1.540940	-0.719175	-5.366436
H	2.509246	-2.169533	-4.922092
C	0.858120	-5.046759	-4.648669
H	1.906453	-4.761942	-4.481047
C	-2.570487	-4.082919	-3.417328
H	-2.313904	-3.312906	-2.677226
C	-0.796312	-6.416024	-5.800041
H	-1.054078	-7.202116	-6.526163
C	-3.895868	-4.423066	-3.647166
H	-4.695281	-3.912289	-3.092881
C	-0.968862	-0.766659	-3.391159
H	-1.483853	-0.789799	-2.410012
H	-0.719624	0.286231	-3.635738
H	-1.658242	-1.149434	-4.170460
C	0.526397	-6.063778	-5.579938
H	1.334919	-6.569333	-6.130071
C	-3.218832	-6.089930	-5.289788
H	-3.469493	-6.876715	-6.018435
C	-4.220695	-5.433791	-4.590222
H	-5.275693	-5.696088	-4.762428

FUDNIB

Conformation 18.
Multiplicity: 5
Charge: 0
E(B97-3c) = -4543.371079649190 Hartree
E(M06/def2-TZVP) = -4543.374218507835 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -4541.719550568001 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -4542.045812467126 Hartree
E(PBEh-3c) = -4537.456637886689 Hartree
E(PM6) = 211.25911 Kcal/mol
E(PM7) = -4.53441 Kcal/mol

E(ωB97X-V/def2-TZVP) = -4545.914083603027 Hartree
E(GFN1-xTB) = -154.671473112078 Hartree
E(GFN2-xTB) = -153.632770400669 Hartree
E(GFN-FF) = -21.588826957928 Hartree

Coordinates:

Fe	0.376637	-0.072395	0.898803
Si	1.117302	3.188491	0.988490
Si	-0.298077	1.479881	3.174612
Si	-1.343653	-1.020482	-1.637776
Si	1.515941	-2.163653	-0.904737
N	0.573749	1.668078	1.669572
N	0.115505	-1.131469	-0.673439
C	-0.196318	3.844085	-0.207103
C	-0.658339	5.177688	-0.203694
C	-1.663762	5.596072	-1.091080
C	-2.216096	4.689395	-2.010937
C	-1.765089	3.359242	-2.037548
C	-0.774702	2.948788	-1.133657
C	2.711717	2.858866	0.004651
C	3.965969	2.821081	0.655634
C	5.135072	2.453159	-0.028983
C	5.074324	2.116475	-1.390966
C	3.844384	2.176235	-2.065680
C	2.680631	2.552780	-1.375133
C	1.460531	4.469275	2.335968
C	-1.744061	2.688311	3.326833
C	-2.076229	3.312759	4.550462
C	-3.135156	4.231259	4.631769
C	-3.882518	4.544591	3.484865
C	-3.568647	3.935472	2.259241
C	-2.510096	3.018041	2.184504
C	-2.705035	-0.142701	-0.662276
C	2.505795	-1.876210	0.701584
C	2.991122	-0.575535	1.000022
C	3.596891	-0.297312	2.241713
C	3.758851	-1.318059	3.188090
C	3.330463	-2.625395	2.887811
C	2.708358	-2.896229	1.660341
C	2.616330	-1.681294	-2.363718
H	-0.239350	5.904063	0.510795
H	-2.018944	6.638165	-1.065003
H	-2.998721	5.020651	-2.711026
H	-2.178098	2.636623	-2.758431
H	-0.447543	1.897417	-1.142957
H	4.034226	3.077917	1.725798
H	6.098653	2.423612	0.503083
H	5.987396	1.817417	-1.928128
H	3.791154	1.932155	-3.138512
H	1.728073	2.613376	-1.922895
H	2.233156	4.108297	3.044478
H	0.539289	4.682247	2.915942
H	1.822956	5.420965	1.896729
H	-1.495476	3.084157	5.458675
H	-3.376095	4.709070	5.594153
H	-4.708938	5.269587	3.546204
H	-4.139746	4.183563	1.351469
H	-2.261175	2.568505	1.211643
H	-3.040552	-0.756142	0.195998
H	-3.577148	0.055994	-1.317951
H	-2.357138	0.830558	-0.263064
H	2.945941	0.227194	0.245637
H	3.945828	0.723220	2.453960
H	4.232293	-1.101719	4.158205
H	3.474820	-3.433167	3.622063
H	2.359332	-3.917204	1.437367
H	2.073736	-1.744165	-3.328294
H	3.505517	-2.342602	-2.415020
H	2.981417	-0.641511	-2.239727
C	0.816903	1.563760	4.697556
H	1.671972	0.870998	4.559915
H	1.223705	2.585277	4.839334
H	0.278960	1.268661	5.621575
C	1.085238	-4.003171	-1.007358
C	-0.005499	-4.514910	-0.268949
C	1.829728	-4.904288	-1.799500
C	-0.342198	-5.874549	-0.318794
C	1.497349	-6.267823	-1.854427
C	0.409712	-6.755209	-1.113649
H	-0.616119	-3.825424	0.332194
H	2.682334	-4.539082	-2.393981
H	-1.207584	-6.246740	0.251072
H	2.087748	-6.952723	-2.482937
H	0.142491	-7.822277	-1.161496
C	-0.962785	-0.302149	2.984174
C	-2.345440	-0.591821	2.830454
C	-0.048991	-1.400279	3.007316
C	-2.796856	-1.906706	2.674718
C	-0.513082	-2.724281	2.842928
C	-1.877645	-2.976240	2.668190
H	-3.069647	0.238230	2.830640
H	1.013876	-1.240867	3.254204
H	-3.873379	-2.107679	2.559671
H	0.207167	-3.554804	2.861908
H	-2.235303	-4.009521	2.540775
C	-1.983242	-2.727617	-2.156876
C	-3.035242	-3.372018	-1.470051
C	-1.351874	-3.429864	-3.208341
C	-3.436345	-4.673342	-1.811996
C	-1.737403	-4.734603	-3.546907
C	-2.782137	-5.359506	-2.847083
H	-3.548244	-2.854163	-0.643585
H	-0.533625	-2.948196	-3.768839
H	-4.260538	-5.157245	-1.264590
H	-1.218128	-5.269745	-4.356595
H	-3.085954	-6.384755	-3.109229
C	-1.016960	-0.038247	-3.231240
C	-2.024863	0.088617	-4.214793
C	0.204162	0.633201	-3.447379
C	-1.824485	0.872086	-5.362165
C	0.413493	1.418274	-4.592178
C	-0.603735	1.542549	-5.551002
H	-2.984673	-0.439154	-4.084049
H	0.997287	0.547493	-2.690346
H	-2.623072	0.960340	-6.115333
H	1.372615	1.941216	-4.734106
H	-0.446353	2.160762	-6.448276

Conformation 2.
Multiplicity: 5
Charge: 0
E(B97-3c) = -4543.368423474888 Hartree
E(M06/def2-TZVP) = -4543.373174660177 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -4541.717326316109 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -4542.044023654015 Hartree
E(PBEh-3c) = -4537.456736584071 Hartree
E(PM6) = 209.06869 Kcal/mol
E(PM7) = -3.64883 Kcal/mol
E(ωB97X-V/def2-TZVP) = -4545.917892854042 Hartree
E(GFN1-xTB) = -154.668709757897 Hartree
E(GFN2-xTB) = -153.625767829555 Hartree
E(GFN-FF) = -21.594184897013 Hartree

Coordinates:

Fe	0.631272	-0.563765	0.017905
Si	-0.288124	2.626766	-0.557936
Si	2.567212	1.390641	-0.489757
Si	-0.475642	-3.566304	-0.324298
Si	-1.317444	-1.743247	2.021299
N	0.819029	1.267384	-0.445150
N	-0.409671	-2.055397	0.557942
C	-1.604740	2.237051	-1.867608
C	-1.290077	1.377998	-2.943028
C	-2.218113	1.105699	-3.960655
C	-3.487310	1.704646	-3.925406
C	-3.816078	2.575946	-2.873871
C	-2.883459	2.836859	-1.856897
C	0.654015	4.157994	-1.181600
C	0.701777	4.457033	-2.563292
C	1.448725	5.541495	-3.048837
C	2.161560	6.358704	-2.156265
C	2.117816	6.087381	-0.779649
C	1.369521	5.000634	-0.300249
C	-1.114763	3.014807	1.091273
C	3.247208	2.544893	0.840331
C	2.607209	2.604132	2.099023
C	3.065285	3.472301	3.102185
C	4.179403	4.294673	2.865264
C	4.832691	4.242174	1.623048
C	4.367498	3.375106	0.621726
C	0.585058	-4.912764	0.473077
C	-0.262869	-0.579420	3.095790
C	-0.800871	0.552894	3.747971
C	-0.032137	1.301609	4.653490
C	1.293120	0.925932	4.929274
C	1.852959	-0.185006	4.278368
C	1.081883	-0.926486	3.369676
C	-1.630888	-3.312737	3.031163
H	-0.288449	0.921494	-2.972304
H	-1.953821	0.423312	-4.783719
H	-4.219914	1.495776	-4.720106
H	-4.808577	3.052086	-2.844570
H	-3.163001	3.516958	-1.036411
H	0.140794	3.829041	-3.274182
H	1.471181	5.753256	-4.129147
H	2.747072	7.211197	-2.534505
H	2.674637	6.721288	-0.072447
H	1.362114	4.798857	0.782043
H	-0.357717	3.260196	1.862298
H	-1.694620	2.140984	1.447672
H	-1.802831	3.879720	0.999359
H	1.731409	1.965915	2.296132

H	2.548233	3.505569	4.073421
H	4.540892	4.976614	3.650891
H	5.706550	4.884688	1.432484
H	4.879746	3.359158	-0.353131
H	1.617091	-4.538652	0.617061
H	0.628246	-5.837768	-0.137845
H	0.175941	-5.181295	1.467522
H	-1.845039	0.845253	3.551772
H	-0.471506	2.179137	5.153085
H	1.893170	1.501850	5.650486
H	2.895468	-0.475040	4.482285
H	1.529797	-1.801524	2.870801
H	-2.251236	-4.034330	2.462275
H	-2.154197	-3.070851	3.978258
H	-0.669281	-3.796296	3.295980
C	3.262294	1.803553	-2.191758
H	2.817367	1.130678	-2.953180
H	3.016651	2.846661	-2.474382
H	4.363142	1.672319	-2.219920
C	-2.978319	-0.894467	1.684199
C	-3.193059	-0.120212	0.522748
C	-4.049563	-1.022947	2.597343
C	-4.431139	0.492728	0.274094
C	-5.289294	-0.409823	2.359186
C	-5.482900	0.346839	1.192987
H	-2.381583	-0.001766	-0.214814
H	-3.920986	-1.620333	3.513983
H	-4.569708	1.082290	-0.643844
H	-6.109328	-0.530363	3.084121
H	-6.456460	0.823207	0.999213
C	3.094266	-0.395688	-0.027465
C	3.707451	-0.711098	1.214766
C	2.948069	-1.445351	-0.980285
C	4.137831	-2.011606	1.502278
C	3.388321	-2.752893	-0.690645
C	3.976468	-3.035791	0.548390
H	3.844618	0.086746	1.960472
H	2.552332	-1.233829	-1.986344
H	4.609653	-2.232499	2.472434
H	3.272924	-3.541921	-1.447579
H	4.325560	-4.056033	0.770915
C	0.173348	-3.202957	-2.073705
C	-0.056025	-1.941279	-2.668520
C	0.920171	-4.147670	-2.811320
C	0.464556	-1.622624	-3.933950
C	1.444157	-3.838608	-4.076924
C	1.224272	-2.569742	-4.638115
H	-0.656149	-1.185318	-2.130212
H	1.113769	-5.144663	-2.383865
H	0.279177	-0.630652	-4.373481
H	2.030068	-4.590086	-4.628970
H	1.638475	-2.321116	-5.627118
C	-2.261307	-4.192332	-0.448544
C	-2.631203	-5.497825	-0.054537
C	-3.277696	-3.330304	-0.919665
C	-3.966222	-5.928002	-0.124972
C	-4.613943	-3.750119	-0.984656
C	-4.960723	-5.052180	-0.588200
H	-1.865570	-6.195129	0.321917
H	-3.024236	-2.304774	-1.229930
H	-4.232041	-6.949784	0.188734
H	-5.389889	-3.052799	-1.337233
H	-6.008972	-5.384977	-0.638550

Conformation 21.
Multiplicity: 5
Charge: 0
E(B97-3c) = -4543.367091138188 Hartree
E(M06/def2-TZVP) = -4543.371282237613 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -4541.717394545529 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -4542.042593890112 Hartree
E(PBEh-3c) = -4537.452805720653 Hartree
E(PM6) = 217.16784 Kcal/mol
E(PM7) = -3.22646 Kcal/mol
E(ωB97X-V/def2-TZVP) = -4545.913271856990 Hartree
E(GFN1-xTB) = -154.672058260097 Hartree
E(GFN2-xTB) = -153.626863228533 Hartree
E(GFN-FF) = -21.456172761762 Hartree

Coordinates:

Fe	-0.549608	0.606329	0.378808
Si	2.234839	-0.462468	-1.002214
Si	1.061394	2.516232	-0.898110
Si	-2.545359	-1.663011	0.591133
Si	-1.732991	-0.067501	3.204537
N	1.062057	0.786006	-0.626295
N	-1.645314	-0.478986	1.510025
C	3.942445	0.327563	-1.290134
C	4.536362	0.470396	-2.564019
C	5.771816	1.119070	-2.725282
C	6.449796	1.632316	-1.608913
C	5.888413	1.486701	-0.329585
C	4.651430	0.842693	-0.179003
C	1.699327	-1.447589	-2.533152
C	1.584508	-0.827247	-3.800146
C	1.152994	-1.542693	-4.927568
C	0.808216	-2.899695	-4.809016
C	0.902754	-3.531748	-3.559531
C	1.349338	-2.814307	-2.437274
C	2.366076	-1.651340	0.459355
C	0.933128	2.939832	-2.739238
C	0.080723	2.171088	-3.563176
C	-0.069137	2.457671	-4.927826
C	0.646931	3.520607	-5.502537
C	1.507612	4.291059	-4.703939
C	1.645532	4.003780	-3.335972
C	-4.200354	-2.112060	1.388829
C	-1.446355	-1.595470	4.300251
C	-0.137192	-2.067475	4.553789
C	0.085041	-3.251387	5.273570
C	-1.004369	-3.989872	5.764132
C	-2.311696	-3.530177	5.541606
C	-2.525847	-2.343828	4.821135
C	-3.368749	0.749959	3.678487
H	4.030083	0.060357	-3.450929
H	6.209770	1.220164	-3.730550
H	7.418898	2.139834	-1.733538
H	6.416870	1.878439	0.553633
H	4.223757	0.745368	0.832465
H	1.817120	0.242680	-3.910763
H	1.075850	-1.033819	-5.901576
H	0.463661	-3.462670	-5.690304
H	0.620697	-4.590009	-3.449615
H	1.398901	-3.333929	-1.467320
H	1.372787	-2.070982	0.716958
H	2.765237	-1.132184	1.353814
H	3.045458	-2.497997	0.234014
H	-0.459280	1.313217	-3.134309
H	-0.741472	1.840885	-5.545461
H	0.538495	3.747653	-6.574481
H	2.077234	5.120500	-5.151212
H	2.326045	4.619704	-2.726810
H	-4.020989	-2.574231	2.380237
H	-4.743590	-2.848531	0.762753
H	-4.849076	-1.223963	1.528411
H	0.728652	-1.498098	4.178937
H	1.114057	-3.599050	5.455236
H	-0.833642	-4.920948	6.326404
H	-3.170035	-4.098922	5.932067
H	-3.560077	-1.996802	4.663245
H	-3.514766	1.651355	3.050628
H	-3.396101	1.046519	4.746979
H	-4.222156	0.067549	3.494701
C	2.460037	3.516769	-0.129679
H	2.568392	3.281388	0.946159
H	3.421882	3.291434	-0.630211
H	2.255138	4.602780	-0.228745
C	-0.305928	1.144858	3.520059
C	-0.437205	2.258594	4.378424
C	0.950461	0.933827	2.904402
C	0.637869	3.130334	4.610679
C	2.031909	1.800660	3.133733
C	1.877466	2.902375	3.988772
H	-1.402298	2.456510	4.871063
H	1.093007	0.067962	2.235819
H	0.510399	3.994558	5.281238
H	2.999948	1.610767	2.645303
H	2.723108	3.583065	4.171886
C	-0.584517	2.971117	-0.016266
C	-1.836927	2.529485	-0.550391
C	-0.613124	3.763676	1.164692
C	-3.050932	2.861696	0.092114
C	-1.819382	4.094453	1.788508
C	-3.043072	3.640654	1.253661
H	-1.884732	2.017151	-1.525420
H	0.332949	4.107872	1.609815
H	-4.000569	2.517120	-0.342375
H	-1.810430	4.703642	2.705004
H	-3.991824	3.909791	1.743187
C	-1.540385	-3.255184	0.349321
C	-0.594171	-3.642996	1.324090
C	-1.737662	-4.112828	-0.757062
C	0.137688	-4.834043	1.197152
C	-1.009546	-5.305936	-0.890033
C	-0.065240	-5.667529	0.085371
H	-0.431214	-3.002997	2.204190
H	-2.466298	-3.841473	-1.538056
H	0.869291	-5.111011	1.972389
H	-1.179784	-5.957165	-1.761913
H	0.507340	-6.602377	-0.019209
C	-2.862120	-0.918637	-1.132236
C	-1.930886	-1.077062	-2.185871

C	-4.036486	-0.175815	-1.398606
C	-2.166179	-0.520838	-3.455184
C	-4.268546	0.397996	-2.657642
C	-3.331781	0.223765	-3.691512
H	-1.010431	-1.659181	-2.029483
H	-4.788214	-0.041303	-0.604080
H	-1.428616	-0.681483	-4.255650
H	-5.188887	0.974893	-2.839163
H	-3.515716	0.662360	-4.684577

Conformation 23.
Multiplicity: 5
Charge: 0
E(B97-3c) = -4543.367256545556 Hartree
E(M06/def2-TZVP) = -4543.369366511494 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -4541.715928459251 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -4542.041236006112 Hartree
E(PBEh-3c) = -4537.453376490443 Hartree
E(PM6) = 224.33014 Kcal/mol
E(PM7) = -5.19854 Kcal/mol
E(ωB97X-V/def2-TZVP) = -4545.914275737952 Hartree
E(GFN1-xTB) = -154.668888547662 Hartree
E(GFN2-xTB) = -153.627301352972 Hartree
E(GFN-FF) = -21.586369281711 Hartree

Coordinates:

Fe	0.293224	-0.557382	0.489965
Si	-0.318058	2.729944	0.731852
Si	1.780039	1.025225	2.289629
Si	-1.872455	-1.998980	-0.863010
Si	0.961984	-1.995329	-2.294669
N	0.435890	1.209398	1.179754
N	-0.190058	-1.555752	-1.055108
C	-0.056274	3.061257	-1.117022
C	0.653506	2.161943	-1.939623
C	0.783972	2.376736	-3.320990
C	0.213747	3.518696	-3.904201
C	-0.479728	4.441013	-3.101816
C	-0.614006	4.210426	-1.723668
C	0.487958	4.153474	1.698071
C	1.484314	4.963825	1.106250
C	2.140991	5.963049	1.842084
C	1.810454	6.173110	3.190980
C	0.815074	5.388071	3.794548
C	0.159662	4.393795	3.052190
C	-2.173903	2.718836	1.088950
C	1.242461	1.408441	4.062429
C	-0.085119	1.121742	4.451606
C	-0.541386	1.412067	5.745658
C	0.326904	2.005722	6.677151
C	1.650081	2.298124	6.308429
C	2.102091	1.997789	5.013433
C	-2.351934	-3.640660	-1.660069
C	1.006242	-3.887921	-2.434027
C	0.993390	-4.565607	-3.671414
C	1.011498	-5.969677	-3.727500
C	1.045269	-6.720751	-2.542208
C	1.061539	-6.062827	-1.300196
C	1.039337	-4.661224	-1.250683
C	2.685122	-1.394733	-1.798232
H	1.082488	1.253502	-1.486744
H	1.311728	1.640470	-3.945202
H	0.307233	3.687431	-4.988117
H	-0.924351	5.341002	-3.554884
H	-1.166439	4.940860	-1.109231
H	1.754040	4.804079	0.049628
H	2.915557	6.580993	1.361450
H	2.327652	6.952590	3.771846
H	0.551315	5.544237	4.851933
H	-0.608503	3.781276	3.549522
H	-2.375801	2.438198	2.142542
H	-2.693674	2.004272	0.419911
H	-2.608500	3.723303	0.910490
H	-0.777321	0.685352	3.714923
H	-1.580718	1.181731	6.029333
H	-0.028894	2.242816	7.691773
H	2.332184	2.768480	7.033692
H	3.139523	2.246439	4.738181
H	-2.136556	-3.622941	-2.747399
H	-3.436762	-3.828393	-1.525814
H	-1.784113	-4.489727	-1.231222
H	0.958173	-3.984907	-4.607826
H	0.994053	-6.481349	-4.702538
H	1.055994	-7.820937	-2.585274
H	1.086237	-6.647723	-0.366831
H	1.033950	-4.151448	-0.273317
H	2.735922	-0.291283	-1.691754
H	3.437488	-1.700635	-2.553452
H	2.980393	-1.855017	-0.835411
C	3.352879	1.962516	1.846526
H	3.606364	1.806912	0.778417
H	3.208954	3.048837	2.008112
H	4.212877	1.627799	2.462404
C	0.549000	-1.275897	-4.004023
C	1.577735	-0.884494	-4.892528
C	-0.785774	-1.104063	-4.433789
C	1.287046	-0.329917	-6.149856
C	-1.085287	-0.543095	-5.684498
C	-0.048060	-0.150218	-6.545123
H	2.632164	-1.003303	-4.596500
H	-1.618391	-1.391676	-3.774913
H	2.106897	-0.029536	-6.820880
H	-2.135734	-0.404405	-5.983168
H	-0.280002	0.294340	-7.525309
C	2.117357	-0.854246	2.129496
C	1.113613	-1.802172	2.503030
C	3.372454	-1.360851	1.694178
C	1.365231	-3.189816	2.404426
C	3.616062	-2.735386	1.609450
C	2.605561	-3.655182	1.956263
H	0.178586	-1.469704	2.987016
H	4.170981	-0.656249	1.414835
H	0.584167	-3.900018	2.709381
H	4.597572	-3.100148	1.269845
H	2.798099	-4.736484	1.887043
C	-3.016323	-0.617987	-1.477232
C	-4.421479	-0.716849	-1.352515
C	-2.480987	0.563092	-2.032341
C	-5.258958	0.328572	-1.770144
C	-3.312116	1.613521	-2.454939
C	-4.704229	1.496334	-2.323275
H	-4.873194	-1.621012	-0.910502
H	-1.391202	0.662469	-2.133541
H	-6.351024	0.235440	-1.662608
H	-2.861186	2.524295	-2.877424
H	-5.362057	2.317095	-2.649121
C	-2.161989	-2.092119	1.022767
C	-2.577775	-0.944148	1.740570
C	-1.968617	-3.289527	1.750625
C	-2.769602	-0.983897	3.132053
C	-2.165735	-3.337057	3.139020
C	-2.556343	-2.179572	3.835401
H	-2.776670	-0.008795	1.197252
H	-1.654432	-4.203026	1.219822
H	-3.101399	-0.079832	3.665761
H	-2.015207	-4.281019	3.686096
H	-2.703954	-2.214031	4.925695

Conformation 24.
Multiplicity: 5
Charge: 0
E(B97-3c) = -4543.361856864503 Hartree
E(M06/def2-TZVP) = -4543.365468626444 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -4541.711997926952 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -4542.037069662785 Hartree
E(PBEh-3c) = -4537.447833398744 Hartree
E(PM6) = 215.50676 Kcal/mol
E(PM7) = -3.31226 Kcal/mol
E(ωB97X-V/def2-TZVP) = -4545.912577660856 Hartree
E(GFN1-xTB) = -154.666139085289 Hartree
E(GFN2-xTB) = -153.625652613226 Hartree
E(GFN-FF) = -21.584218918269 Hartree

Coordinates:

Fe	0.495859	0.118908	-0.539992
Si	-0.565781	-2.863932	0.145283
Si	-0.688596	-1.340070	-2.658982
Si	-0.569655	2.186997	1.501566
Si	2.516335	1.760730	1.173960
N	-0.166181	-1.601696	-1.005788
N	0.837062	1.490376	0.734852
C	0.120421	-4.534007	-0.437425
C	1.193269	-4.594910	-1.353168
C	1.756202	-5.821847	-1.739111
C	1.251591	-7.020327	-1.209540
C	0.185294	-6.982930	-0.296082
C	-0.372345	-5.751905	0.083995
C	-2.446936	-3.013032	0.345691
C	-3.132861	-2.213639	1.288390
C	-4.532945	-2.248019	1.389214
C	-5.275846	-3.091716	0.548305
C	-4.613425	-3.897881	-0.391217
C	-3.214867	-3.856400	-0.488915
C	0.184058	-2.452999	1.824000
C	-2.553661	-1.507794	-2.911442
C	-3.455857	-0.851054	-2.043135
C	-4.842050	-0.971492	-2.208520
C	-5.358326	-1.765233	-3.245678
C	-4.481446	-2.433975	-4.112991
C	-3.092830	-2.302712	-3.946923
C	-2.118251	1.623118	0.569847
C	3.262128	0.014555	1.216863

C	3.199017	-0.775195	0.043297
C	3.584986	-2.124501	0.040247
C	4.046836	-2.717193	1.225829
C	4.125190	-1.952510	2.401309
C	3.736935	-0.601490	2.393990
C	2.764909	2.659450	2.814887
H	1.586645	-3.656066	-1.771781
H	2.590130	-5.844252	-2.458336
H	1.687947	-7.985417	-1.510403
H	-0.215801	-7.920211	0.120349
H	-1.213160	-5.739518	0.797101
H	-2.567517	-1.548648	1.962172
H	-5.045387	-1.615845	2.131235
H	-6.374014	-3.119691	0.623603
H	-5.191091	-4.554521	-1.059689
H	-2.710061	-4.488839	-1.236658
H	-0.214452	-1.501980	2.228586
H	1.285954	-2.365634	1.756215
H	-0.056093	-3.257353	2.548819
H	-3.069552	-0.250389	-1.207330
H	-5.522224	-0.458267	-1.512194
H	-6.447071	-1.868564	-3.372909
H	-4.880250	-3.062445	-4.924481
H	-2.420963	-2.836196	-4.637722
H	-2.146320	2.009987	-0.468119
H	-3.030893	1.972990	1.094206
H	-2.162040	0.514123	0.533642
H	2.866184	-0.315290	-0.907409
H	3.517719	-2.717585	-0.883195
H	4.338255	-3.778335	1.232817
H	4.485313	-2.414866	3.333415
H	3.797332	-0.019940	3.328115
H	2.355313	3.686757	2.739240
H	3.850323	2.745538	3.027135
H	2.268254	2.156837	3.666922
C	0.222065	-2.384084	-3.943040
H	1.318965	-2.256460	-3.844125
H	-0.003875	-3.462169	-3.819018
H	-0.062929	-2.076754	-4.970131
C	3.415530	2.774539	-0.152676
C	4.571826	2.317002	-0.821475
C	2.921445	4.058126	-0.481368
C	5.202463	3.103354	-1.801300
C	3.552209	4.851626	-1.450864
C	4.691541	4.372062	-2.119978
H	4.986013	1.325529	-0.577605
H	2.016191	4.440438	0.016744
H	6.099158	2.725277	-2.316864
H	3.149664	5.848859	-1.689311
H	5.184552	4.989832	-2.886525
C	-0.168677	0.492544	-2.865575
C	-1.096780	1.557259	-3.026658
C	1.223997	0.822354	-2.871235
C	-0.663895	2.882689	-3.150371
C	1.654476	2.161838	-2.990827
C	0.711974	3.187683	-3.115975
H	-2.173327	1.327761	-3.061262
H	1.979937	0.019502	-2.904171
H	-1.402654	3.689050	-3.279632
H	2.728545	2.396902	-2.992570
H	1.052615	4.230434	-3.198522
C	-0.486442	4.082728	1.460940
C	-0.612728	4.743087	0.216147
C	-0.221069	4.869674	2.603206
C	-0.475575	6.135709	0.114025
C	-0.079231	6.264227	2.507069
C	-0.205113	6.899778	1.261783
H	-0.800545	4.153053	-0.695321
H	-0.118548	4.382398	3.586361
H	-0.576302	6.628842	-0.865710
H	0.132475	6.858447	3.409623
H	-0.093072	7.992357	1.184995
C	-0.757065	1.593443	3.294500
C	0.079863	0.587282	3.824475
C	-1.786396	2.099104	4.121666
C	-0.099710	0.100820	5.129483
C	-1.970084	1.620679	5.428609
C	-1.125810	0.618541	5.935044
H	0.885643	0.173354	3.198395
H	-2.458579	2.886768	3.741279
H	0.563091	-0.688836	5.516368
H	-2.776620	2.030646	6.056402
H	-1.269926	0.240653	6.959037

Conformation 26.
Multiplicity: 5
Charge: 0
E(B97-3c) = -4543.364960019486 Hartree
E(M06/def2-TZVP) = -4543.368737449843 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -4541.714985452026 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -4542.040417035433 Hartree

E(PBEh-3c) = -4537.450265528681 Hartree
E(PM6) = 208.04060 Kcal/mol
E(PM7) = -5.85628 Kcal/mol
E(ωB97X-V/def2-TZVP) = -4545.910341974219 Hartree
E(GFN1-xTB) = -154.670020074520 Hartree
E(GFN2-xTB) = -153.625932708899 Hartree
E(GFN-FF) = -21.596416885984 Hartree

Coordinates:

Fe	0.022662	-0.139476	0.109807
Si	-0.586809	0.511578	-2.929910
Si	-2.231860	1.813413	-0.642683
Si	1.562970	-2.244027	1.165721
Si	3.044395	0.557279	1.280897
N	-1.028284	0.684748	-1.243694
N	1.686610	-0.501638	0.997152
C	-2.091798	0.013894	-3.966663
C	-2.331694	0.561023	-5.246267
C	-3.454546	0.181788	-5.999677
C	-4.360076	-0.758174	-5.483515
C	-4.137040	-1.316180	-4.214336
C	-3.014901	-0.931778	-3.466404
C	0.724349	-0.856042	-3.116930
C	2.089415	-0.566609	-2.887936
C	3.090803	-1.515801	-3.144148
C	2.743225	-2.787561	-3.628708
C	1.392169	-3.101769	-3.848728
C	0.396788	-2.142767	-3.600462
C	0.164846	2.099172	-3.637031
C	-3.971208	1.459699	-1.307245
C	-4.553556	2.291969	-2.288895
C	-5.804705	1.992649	-2.850856
C	-6.513327	0.858928	-2.425270
C	-5.958169	0.021429	-1.444801
C	-4.697603	0.315298	-0.905005
C	2.696523	-3.250080	0.049750
C	2.788202	2.218174	0.384821
C	3.241883	2.418144	-0.938480
C	3.012754	3.625275	-1.618149
C	2.320830	4.667833	-0.981127
C	1.889476	4.505973	0.345147
C	2.133082	3.298555	1.019711
C	4.663885	-0.195937	0.644722
H	-1.632508	1.302906	-5.664715
H	-3.626335	0.625166	-6.993119
H	-5.245003	-1.052027	-6.069100
H	-4.852079	-2.042505	-3.797840
H	-2.859537	-1.355742	-2.462176
H	2.376004	0.428140	-2.514693
H	4.148391	-1.263646	-2.967403
H	3.525781	-3.534182	-3.833349
H	1.113794	-4.096303	-4.231113
H	-0.656813	-2.391525	-3.804346
H	0.898058	2.523105	-2.921799
H	-0.615807	2.866296	-3.813111
H	0.684290	1.905650	-4.597746
H	-4.015752	3.188476	-2.635319
H	-6.228533	2.647150	-3.628073
H	-7.495723	0.623897	-2.863145
H	-6.504773	-0.874817	-1.110594
H	-4.255402	-0.376204	-0.173817
H	2.583105	-2.954763	-1.010173
H	2.469862	-4.331523	0.148734
H	3.758769	-3.105241	0.328711
H	3.801168	1.618764	-1.449794
H	3.376705	3.753617	-2.649238
H	2.130068	5.611831	-1.513968
H	1.366580	5.326837	0.859958
H	1.819871	3.199045	2.071479
H	4.933133	-1.098203	1.230083
H	5.499634	0.527058	0.736207
H	4.570786	-0.497760	-0.418450
C	-1.762575	3.612062	-0.995113
H	-0.727713	3.792748	-0.638637
H	-1.787482	3.855289	-2.075913
H	-2.445089	4.307878	-0.465219
C	3.252028	0.973170	3.122153
C	2.487478	0.352351	4.133371
C	4.219643	1.926630	3.516322
C	2.684894	0.663083	5.489037
C	4.420196	2.244427	4.868161
C	3.652305	1.609941	5.859161
H	1.727488	-0.392071	3.855693
H	4.824953	2.440564	2.750641
H	2.082066	0.155215	6.257923
H	5.178532	2.990925	5.151702
H	3.810107	1.855546	6.920825
C	-2.143410	1.566412	1.243184
C	-3.204431	1.149453	2.075805
C	-0.874816	1.768911	1.845694
C	-2.996469	0.890949	3.440430

C	-0.661938	1.520679	3.213935
C	-1.721320	1.061459	4.009147
H	-4.211402	1.020592	1.649753
H	-0.045955	2.181560	1.247052
H	-3.837261	0.556876	4.068288
H	0.332435	1.683914	3.654361
H	-1.558021	0.853329	5.077716
C	-0.250329	-2.504931	0.631732
C	-1.313657	-1.887728	1.362928
C	-0.602321	-3.328117	-0.474344
C	-2.660412	-2.119634	1.006906
C	-1.937263	-3.533248	-0.833786
C	-2.972296	-2.933495	-0.086455
H	-1.103298	-1.299410	2.271881
H	0.192683	-3.806273	-1.065782
H	-3.458787	-1.662202	1.609025
H	-2.180385	-4.165973	-1.701190
H	-4.023495	-3.107908	-0.363451
C	1.841508	-2.820988	2.953244
C	3.163133	-2.870136	3.455100
C	0.788297	-3.124171	3.844927
C	3.424456	-3.182584	4.796752
C	1.042465	-3.437807	5.190104
C	2.361315	-3.461369	5.670627
H	4.012227	-2.638954	2.791100
H	-0.252173	-3.117094	3.485291
H	4.461672	-3.200914	5.165209
H	0.205060	-3.668659	5.866938
H	2.561892	-3.702812	6.725875

Conformation 27.
Multiplicity: 5
Charge: 0
E(B97-3c) = -4543.373511532836 Hartree
E(M06/def2-TZVP) = -4543.376078082881 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -4541.722502909398 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -4542.048319576493 Hartree
E(PBEh-3c) = -4537.459303363538 Hartree
E(PM6) = 214.02917 Kcal/mol
E(PM7) = -10.75376 Kcal/mol
E(ωB97X-V/def2-TZVP) = -4545.914376560694 Hartree
E(GFN1-xTB) = -154.673473282311 Hartree
E(GFN2-xTB) = -153.633378270335 Hartree
E(GFN-FF) = -21.472010168773 Hartree

Coordinates:

Fe	0.094271	-0.453360	-0.303630
Si	-3.053055	-0.241472	-0.155846
Si	-1.238829	-0.597667	2.406487
Si	1.799734	-0.806180	-2.471005
Si	2.105971	2.070796	-1.214833
N	-1.528578	-0.437300	0.689692
N	1.468713	0.443058	-1.287842
C	-2.654459	0.262284	-1.943618
C	-1.844655	1.393129	-2.202951
C	-1.567695	1.810403	-3.514316
C	-2.095468	1.098110	-4.602526
C	-2.896627	-0.032944	-4.369488
C	-3.172578	-0.441162	-3.054878
C	-4.082876	1.124116	0.675519
C	-4.226891	2.418538	0.130008
C	-4.935423	3.421502	0.811972
C	-5.520320	3.147972	2.058211
C	-5.401190	1.862813	2.613353
C	-4.694130	0.864492	1.925490
C	-4.106389	-1.809994	-0.188422
C	-2.353918	-1.921674	3.177306
C	-2.525706	-3.160526	2.517019
C	-3.341304	-4.166232	3.057329
C	-4.013128	-3.948182	4.271571
C	-3.861904	-2.723065	4.940120
C	-3.037534	-1.723525	4.397684
C	1.374118	-0.407995	-4.262565
C	0.731183	3.275805	-0.706762
C	0.477457	4.464785	-1.425563
C	-0.575048	5.324108	-1.065591
C	-1.393694	5.014629	0.031405
C	-1.156778	3.842441	0.767322
C	-0.107843	2.989365	0.395112
C	2.824745	2.599465	-2.883673
H	-1.422716	1.968708	-1.367488
H	-0.934781	2.696571	-3.677230
H	-1.882611	1.421260	-5.633324
H	-3.312208	-0.597137	-5.219064
H	-3.803185	-1.329474	-2.893241
H	-3.772645	2.653382	-0.844957
H	-5.030276	4.423909	0.365420
H	-6.074484	3.933493	2.595039
H	-5.863035	1.636694	3.587237
H	-4.607723	-0.134983	2.383890
H	-4.424481	-2.095868	0.832798
H	-3.536444	-2.658942	-0.615362
H	-5.019919	-1.646842	-0.796539
H	-2.023209	-3.328534	1.551695
H	-3.461465	-5.122794	2.524797
H	-4.658491	-4.733039	4.695393
H	-4.390020	-2.545069	5.889801
H	-2.931606	-0.767879	4.935252
H	0.347617	0.002130	-4.327624
H	1.428366	-1.320157	-4.891881
H	2.072362	0.341799	-4.683081
H	1.105182	4.726574	-2.292295
H	-0.759125	6.239283	-1.649620
H	-2.225493	5.680054	0.309428
H	-1.807756	3.578819	1.613706
H	0.025458	2.050124	0.954525
H	3.615406	1.891410	-3.207216
H	3.286149	3.605762	-2.819420
H	2.042075	2.617705	-3.668649
C	-1.399269	1.014220	3.381217
H	-0.670793	1.763639	3.014317
H	-2.414070	1.447704	3.280607
H	-1.185720	0.847426	4.457041
C	3.492494	2.196804	0.082731
C	4.753321	1.611758	-0.179794
C	3.312730	2.838335	1.328950
C	5.785043	1.642986	0.770910
C	4.340000	2.871272	2.286951
C	5.578118	2.269135	2.011716
H	4.935503	1.107530	-1.141339
H	2.351223	3.325869	1.557129
H	6.754048	1.172235	0.542370
H	4.172554	3.370674	3.253840
H	6.383536	2.291987	2.761989
C	0.578655	-1.169318	2.522132
C	0.938757	-2.488678	2.882228
C	1.626421	-0.265894	2.210056
C	2.280430	-2.899108	2.898619
C	2.974330	-0.667593	2.232437
C	3.300449	-1.989822	2.567644
H	0.150556	-3.207045	3.158229
H	1.409022	0.789508	1.981420
H	2.535115	-3.933164	3.178933
H	3.762185	0.061042	1.993377
H	4.353673	-2.310399	2.582115
C	0.613066	-2.178803	-1.854274
C	-0.519194	-2.603497	-2.605759
C	0.877661	-2.844306	-0.617295
C	-1.348831	-3.630160	-2.147859
C	0.034044	-3.881843	-0.163115
C	-1.073367	-4.272791	-0.922163
H	-0.753752	-2.107934	-3.559615
H	1.799208	-2.629260	-0.051389
H	-2.218373	-3.940216	-2.747657
H	0.267362	-4.388106	0.784830
H	-1.724793	-5.087300	-0.569534
C	3.583085	-1.429255	-2.348196
C	4.337233	-1.822436	-3.476187
C	4.192231	-1.527385	-1.076537
C	5.651693	-2.298012	-3.339322
C	5.501335	-2.009671	-0.932008
C	6.235209	-2.395431	-2.065596
H	3.895102	-1.755115	-4.483363
H	3.637278	-1.195868	-0.185792
H	6.225222	-2.594104	-4.231475
H	5.954006	-2.073676	0.070131
H	7.265153	-2.769425	-1.957730

Conformation 3.
Multiplicity: 5
Charge: 0
E(B97-3c) = -4543.374459280310 Hartree
E(M06/def2-TZVP) = -4543.378788184949 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -4541.721998648313 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -4542.050426495231 Hartree
E(PBEh-3c) = -4537.462565938135 Hartree
E(PM6) = 197.86854 Kcal/mol
E(PM7) = -2.31902 Kcal/mol
E(ωB97X-V/def2-TZVP) = -4545.918446776725 Hartree
E(GFN1-xTB) = -154.674435226022 Hartree
E(GFN2-xTB) = -153.633782870437 Hartree
E(GFN-FF) = -21.591039594908 Hartree

Coordinates:

Fe	0.243001	0.299894	0.414860
Si	-0.349691	2.810784	-1.014597
Si	-2.585466	0.696002	-1.252314
Si	1.564375	-2.534421	-0.390110
Si	1.324981	-1.455849	2.540258
N	-1.047330	1.254927	-0.614003
N	1.177305	-1.316369	0.806669
C	1.445887	2.719151	-0.382264

C	1.981221	3.672186	0.515400
C	3.303778	3.578856	0.971578
C	4.131457	2.533887	0.521925
C	3.636180	1.602298	-0.400384
C	2.305032	1.690367	-0.850419
C	-1.221906	4.218101	-0.096140
C	-2.065467	3.933081	1.000106
C	-2.700538	4.961711	1.713437
C	-2.497620	6.301488	1.344579
C	-1.660048	6.606395	0.259291
C	-1.031911	5.572255	-0.453373
C	-0.257788	3.196419	-2.864768
C	-2.414460	-0.262048	-2.888180
C	-2.398402	-1.675400	-2.927063
C	-2.246910	-2.369988	-4.138328
C	-2.109243	-1.663503	-5.342785
C	-2.133426	-0.259032	-5.329947
C	-2.287461	0.428524	-4.115992
C	2.932384	-3.702078	0.199283
C	3.139808	-1.327182	3.066865
C	4.087499	-0.818753	2.152126
C	5.434521	-0.660088	2.513195
C	5.859286	-1.012323	3.804223
C	4.931469	-1.519603	4.729107
C	3.585359	-1.672748	4.362002
C	0.531240	-2.989410	3.306781
H	1.342545	4.499442	0.864296
H	3.695200	4.323326	1.682044
H	5.166725	2.453508	0.886968
H	4.281495	0.801347	-0.789222
H	1.956209	0.973881	-1.610976
H	-2.222065	2.883327	1.294121
H	-3.360841	4.716714	2.560264
H	-2.995675	7.110186	1.901522
H	-1.499515	7.655133	-0.035508
H	-0.381190	5.829594	-1.305435
H	-1.253037	3.422119	-3.296828
H	0.174996	2.331371	-3.406750
H	0.398457	4.073502	-3.039616
H	-2.493612	-2.250577	-1.994150
H	-2.228295	-3.469954	-4.130520
H	-1.985871	-2.205848	-6.293005
H	-2.034977	0.303508	-6.271741
H	-2.308102	1.529413	-4.131823
H	3.867146	-3.159408	0.444049
H	3.153573	-4.456349	-0.583169
H	2.615062	-4.246555	1.111385
H	3.750435	-0.542974	1.141005
H	6.157462	-0.260893	1.783916
H	6.915366	-0.892572	4.091676
H	5.260689	-1.797929	5.742398
H	2.871592	-2.068623	5.103165
H	-0.550471	-3.042971	3.071522
H	0.649061	-2.997235	4.409951
H	1.004450	-3.909866	2.909956
C	-3.770487	2.140603	-1.571496
H	-3.984484	2.686125	-0.631944
H	-3.370767	2.875169	-2.299670
H	-4.726011	1.748857	-1.976204
C	0.403028	0.095818	3.143855
C	-0.760869	0.027089	3.946489
C	0.878765	1.383532	2.768497
C	-1.446093	1.184833	4.337862
C	0.184681	2.546546	3.158809
C	-0.977121	2.448027	3.934612
H	-1.138348	-0.955646	4.269147
H	1.847101	1.489922	2.250392
H	-2.352349	1.104962	4.957890
H	0.563289	3.533718	2.860110
H	-1.515178	3.360763	4.231444
C	-3.415591	-0.459518	0.000906
C	-4.577015	-1.180612	-0.360845
C	-2.945363	-0.590899	1.323289
C	-5.237199	-2.007130	0.560694
C	-3.594660	-1.422492	2.250394
C	-4.743915	-2.133016	1.870613
H	-4.969288	-1.104084	-1.388326
H	-2.045770	-0.035573	1.639278
H	-6.138624	-2.560944	0.255379
H	-3.205345	-1.508847	3.276244
H	-5.257753	-2.783224	2.595532
C	2.119924	-1.677822	-1.987627
C	3.484462	-1.450775	-2.277152
C	1.158409	-1.168509	-2.890351
C	3.874676	-0.723647	-3.413656
C	1.541109	-0.438480	-4.027729
C	2.902165	-0.210383	-4.288124
H	4.260128	-1.844338	-1.599671
H	0.087748	-1.340209	-2.707919
H	4.943390	-0.554678	-3.619104
H	0.766066	-0.057200	-4.710034
H	3.207546	0.363065	-5.176954
C	0.014857	-3.557035	-0.776730
C	-0.006303	-4.472830	-1.852978
C	-1.142150	-3.449510	0.023402
C	-1.139770	-5.258292	-2.113648
C	-2.281131	-4.231344	-0.229387
C	-2.280136	-5.139147	-1.300141
H	0.875366	-4.566568	-2.508957
H	-1.161630	-2.719642	0.845990
H	-1.137374	-5.965425	-2.958137
H	-3.173904	-4.112673	0.402731
H	-3.172014	-5.750689	-1.507284

Conformation 32.
Multiplicity: 5
Charge: 0
E(B97-3c) = -4543.373696662202 Hartree
E(M06/def2-TZVP) = -4543.376943832447 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -4541.722651042367 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -4542.048818394396 Hartree
E(PBEh-3c) = -4537.460054167191 Hartree
E(PM6) = 210.61454 Kcal/mol
E(PM7) = -10.93816 Kcal/mol
E(ωB97X-V/def2-TZVP) = -4545.915305330425 Hartree
E(GFN1-xTB) = -154.673326112272 Hartree
E(GFN2-xTB) = -153.632637687937 Hartree
E(GFN-FF) = -21.613717693457 Hartree

Coordinates:

Fe	0.028378	-0.357655	-0.372483
Si	0.246205	-2.084556	2.231529
Si	2.223320	0.308302	1.636357
Si	-2.451292	1.739544	-1.147839
Si	-1.352943	-0.738386	-2.764696
N	0.886975	-0.761903	1.272987
N	-1.345588	0.418111	-1.451467
C	-1.420053	-2.579202	1.462102
C	-2.442553	-1.617629	1.281080
C	-3.692625	-1.969374	0.747467
C	-3.948560	-3.299457	0.380190
C	-2.946123	-4.270842	0.544659
C	-1.699330	-3.911501	1.080299
C	-0.020873	-1.514978	4.026015
C	-1.291621	-1.198372	4.554316
C	-1.434059	-0.703931	5.861444
C	-0.303172	-0.518732	6.672038
C	0.969493	-0.841192	6.171871
C	1.104563	-1.337328	4.865935
C	1.370260	-3.602085	2.270970
C	3.754216	-0.672358	2.174240
C	4.135680	-1.819613	1.439998
C	5.261442	-2.574965	1.801250
C	6.027221	-2.201862	2.918135
C	5.661896	-1.071250	3.665841
C	4.538524	-0.314434	3.293320
C	-4.067551	1.513973	-2.104013
C	-0.926153	0.080377	-4.418230
C	0.003735	1.144610	-4.445563
C	0.378176	1.752431	-5.653066
C	-0.181714	1.311375	-6.863155
C	-1.114282	0.261249	-6.857319
C	-1.478658	-0.348537	-5.645776
C	-2.899046	-1.800270	-2.949711
H	-2.268645	-0.571688	1.568796
H	-4.464563	-1.194543	0.622283
H	-4.928237	-3.581312	-0.036040
H	-3.140201	-5.315868	0.256305
H	-0.926268	-4.686637	1.199186
H	-2.190299	-1.335292	3.933197
H	-2.436292	-0.462213	6.249396
H	-0.412925	-0.129223	7.696053
H	1.861491	-0.706812	6.803735
H	2.113791	-1.577428	4.491346
H	2.332896	-3.366782	2.764361
H	1.592634	-3.951308	1.242955
H	0.889007	-4.426038	2.837163
H	3.521958	-2.135555	0.582168
H	5.538464	-3.465770	1.215687
H	6.907588	-2.795692	3.208858
H	6.255519	-0.777570	4.545565
H	4.266310	0.567912	3.894243
H	-3.867657	1.431049	-3.192284
H	-4.742154	2.381317	-1.954769
H	-4.596998	0.593888	-1.783770
H	0.423616	1.518546	-3.499549
H	1.104087	2.580904	-5.647721
H	0.105866	1.788845	-7.812731
H	-1.560474	-0.083983	-7.803013
H	-2.210067	-1.172759	-5.661115
H	-3.184672	-2.234455	-1.971571
H	-2.721096	-2.632270	-3.661834

H	-3.751897	-1.202290	-3.326412
C	1.832959	1.629517	2.929949
H	1.014645	2.290910	2.583468
H	1.517047	1.167903	3.886365
H	2.718364	2.271372	3.117035
C	0.104963	-1.866703	-2.244323
C	1.434617	-1.344797	-2.263224
C	-0.064966	-3.233484	-1.887654
C	2.535855	-2.166448	-1.940713
C	1.030562	-4.039140	-1.563568
C	2.336432	-3.506388	-1.591878
H	1.629089	-0.322500	-2.627868
H	-1.077121	-3.664061	-1.856781
H	3.551071	-1.746104	-1.983556
H	0.872541	-5.094021	-1.290784
H	3.197482	-4.147853	-1.348230
C	2.596552	1.185726	-0.015999
C	3.734221	0.879006	-0.797656
C	1.694595	2.154426	-0.522942
C	3.943899	1.483746	-2.046458
C	1.901505	2.771122	-1.769688
C	3.023689	2.426242	-2.537653
H	4.469759	0.151891	-0.418753
H	0.824210	2.474291	0.071462
H	4.834836	1.224677	-2.639722
H	1.183974	3.522733	-2.129283
H	3.188442	2.900340	-3.517672
C	-1.686389	3.400773	-1.672169
C	-1.549301	3.708743	-3.045981
C	-1.218903	4.350433	-0.736089
C	-0.945327	4.902657	-3.469398
C	-0.611109	5.546938	-1.152281
C	-0.468068	5.823456	-2.521352
H	-1.907985	2.998763	-3.807202
H	-1.332488	4.153236	0.341899
H	-0.843856	5.112893	-4.545682
H	-0.247185	6.267351	-0.403320
H	0.010581	6.758861	-2.850081
C	-2.821506	1.828094	0.711300
C	-4.141479	1.849340	1.212733
C	-1.766957	1.820028	1.653945
C	-4.396737	1.849090	2.595123
C	-2.009160	1.824129	3.034996
C	-3.331218	1.835931	3.508457
H	-4.993183	1.853924	0.513906
H	-0.723902	1.766676	1.303742
H	-5.435458	1.853830	2.960573
H	-1.167703	1.791636	3.742394
H	-3.526697	1.824718	4.591770

Conformation 5.
Multiplicity: 5
Charge: 0
E(B97-3c) = -4543.364294641642 Hartree
E(M06/def2-TZVP) = -4543.369541128376 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -4541.714858146132 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -4542.039604271005 Hartree
E(PBEh-3c) = -4537.450386252622 Hartree
E(PM6) = 210.47233 Kcal/mol
E(PM7) = -2.08331 Kcal/mol
E(ωB97X-V/def2-TZVP) = -4545.913181392230 Hartree
E(GFN1-xTB) = -154.667415494971 Hartree
E(GFN2-xTB) = -153.622833951079 Hartree
E(GFN-FF) = -21.452200643952 Hartree

Coordinates:

Fe	-0.432185	-0.190236	0.559097
Si	1.228972	2.549288	-0.206720
Si	-1.859078	2.225320	0.540553
Si	0.566195	-2.533208	-1.362706
Si	0.678076	-2.803744	1.716878
N	-0.221046	1.684406	0.255525
N	0.207126	-1.956829	0.251916
C	2.145300	3.176695	1.337545
C	3.435108	2.703477	1.667789
C	4.088521	3.113683	2.842087
C	3.465084	4.021751	3.712021
C	2.186701	4.515196	3.400453
C	1.537886	4.090595	2.230798
C	0.812884	4.025639	-1.323437
C	0.268529	3.781933	-2.606414
C	-0.098375	4.835925	-3.454952
C	0.074452	6.165844	-3.038556
C	0.628496	6.431979	-1.777221
C	0.996876	5.371249	-0.932991
C	2.365494	1.365664	-1.139820
C	-2.672007	3.052513	-0.947328
C	-2.642655	2.412269	-2.206383
C	-3.243264	2.995742	-3.330423
C	-3.867471	4.248941	-3.221795
C	-3.894107	4.908238	-1.983209
C	-3.307356	4.309617	-0.856375
C	2.395069	-2.496396	-1.837986
C	2.428365	-3.509726	1.529751
C	2.618943	-4.815582	1.022258
C	3.904547	-5.307050	0.745687
C	5.029969	-4.500741	0.980070
C	4.862845	-3.207055	1.501024
C	3.574999	-2.720704	1.772318
C	-0.471504	-4.213092	2.224509
H	3.944488	1.992068	0.998999
H	5.090336	2.722404	3.078886
H	3.974541	4.345751	4.632605
H	1.691275	5.230349	4.075920
H	0.528483	4.472586	2.015746
H	0.112942	2.746961	-2.951077
H	-0.531514	4.617997	-4.443454
H	-0.220637	6.995305	-3.699992
H	0.778163	7.472779	-1.448870
H	1.443245	5.600424	0.047233
H	1.847853	1.007402	-2.051095
H	2.619518	0.475632	-0.528288
H	3.307002	1.862398	-1.448900
H	-2.126587	1.446245	-2.314702
H	-3.211921	2.474063	-4.299041
H	-4.330525	4.715488	-4.105275
H	-4.375261	5.894752	-1.894133
H	-3.341573	4.840505	0.108040
H	2.808289	-1.473422	-1.740272
H	2.536275	-2.821602	-2.889376
H	2.989259	-3.163837	-1.184442
H	1.748780	-5.458019	0.814743
H	4.027550	-6.323514	0.340309
H	6.039113	-4.882079	0.759854
H	5.742516	-2.573805	1.695047
H	3.461722	-1.704032	2.181200
H	-1.520321	-3.864118	2.293067
H	-0.164158	-4.634076	3.204312
H	-0.443496	-5.029438	1.477284
C	-2.066129	3.303674	2.078889
H	-1.493338	2.875074	2.925871
H	-1.690482	4.332127	1.900649
H	-3.132962	3.373032	2.374990
C	0.631419	-1.458855	3.063022
C	-0.058500	-1.652298	4.282310
C	1.214735	-0.185662	2.837485
C	-0.193901	-0.617725	5.220291
C	1.090901	0.854307	3.777123
C	0.374509	0.642433	4.963161
H	-0.512205	-2.632013	4.499702
H	1.800876	0.002070	1.922117
H	-0.747423	-0.792566	6.156197
H	1.553310	1.829313	3.577079
H	0.268793	1.458857	5.694122
C	-2.690344	0.526731	0.865652
C	-3.624744	-0.084127	-0.016421
C	-2.370258	-0.164586	2.078023
C	-4.183317	-1.333715	0.268425
C	-2.946817	-1.424523	2.360170
C	-3.836828	-2.012150	1.456507
H	-3.911935	0.441454	-0.939570
H	-1.760573	0.324116	2.856807
H	-4.903369	-1.786417	-0.430878
H	-2.701722	-1.925514	3.307559
H	-4.286439	-2.990978	1.684194
C	-0.388203	-1.463256	-2.616841
C	0.279058	-0.708395	-3.608196
C	-1.801993	-1.482155	-2.650959
C	-0.429842	-0.010137	-4.599604
C	-2.517878	-0.799571	-3.645909
C	-1.831801	-0.068377	-4.629490
H	1.379579	-0.677662	-3.621903
H	-2.359266	-2.055072	-1.894763
H	0.116090	0.568866	-5.360588
H	-3.618298	-0.835795	-3.654074
H	-2.390404	0.457920	-5.418805
C	-0.078704	-4.315661	-1.524767
C	-1.360446	-4.650496	-1.028318
C	0.681864	-5.343278	-2.125492
C	-1.866986	-5.954758	-1.133762
C	0.185170	-6.653338	-2.229463
C	-1.092449	-6.961260	-1.735095
H	-1.964258	-3.878213	-0.524348
H	1.688264	-5.122952	-2.515100
H	-2.867804	-6.191563	-0.738342
H	0.798626	-7.438977	-2.698986
H	-1.483471	-7.987780	-1.814718

FUHWAG

Conformation 14.

Multiplicity: 2
Charge: 0
E(B97-3c) = -5613.021580151656 Hartree
E(M06/def2-TZVP) = -5612.879251329144 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -5610.938177584495 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -5611.171797824234 Hartree
E(PBEh-3c) = -5604.822709670281 Hartree
E(PM6) = 180.72323 Kcal/mol
E(PM7) = 67.30399 Kcal/mol
E(ωB97X-V/def2-TZVP) = -5614.579160365128 Hartree
E(GFN1-xTB) = -265.539275425151 Hartree
E(GFN2-xTB) = -259.271386044267 Hartree
E(GFN-FF) = -33.821492421922 Hartree

Coordinates:

Cu	-1.360647	0.573347	0.442464
N	-0.811586	2.417758	1.091880
N	-1.778689	1.329365	-1.393860
N	-1.833886	-1.291849	-0.228677
N	-0.868227	-0.199834	2.252303
C	-0.277515	2.740294	2.322166
C	-0.798179	3.580142	0.349960
C	-1.730559	2.659488	-1.760648
C	-2.190202	0.635978	-2.513822
C	-2.191013	-1.638867	-1.518277
C	-1.707832	-2.476606	0.462854
C	-0.947989	-1.523915	2.629408
C	-0.456357	0.496160	3.370872
C	0.100713	4.142451	2.350568
C	-0.227729	4.664288	1.125968
C	-2.153813	2.812592	-3.138533
C	-2.418267	1.552655	-3.613918
C	-2.333760	-3.078107	-1.627848
C	-2.023812	-3.598486	-0.399521
C	-0.624862	-1.662221	4.035126
C	-0.330132	-0.405376	4.499923
C	-1.247460	3.725341	-0.974719
C	-2.347511	-0.760863	-2.607336
C	-1.266685	-2.608255	1.791624
C	-0.123276	1.864270	3.415633
O	2.073226	4.693643	-4.614880
O	1.269341	-3.169770	-5.223627
O	1.091408	-2.797257	0.250964
O	-2.424256	4.929674	6.812225
N	0.831618	4.125412	-2.763265
N	-0.210090	-1.994077	-3.882787
N	3.223957	-3.104645	-3.174743
N	5.288475	-3.763083	-3.828662
N	1.453020	-3.598845	2.369927
N	-1.592656	3.640054	5.074352
N	-3.769051	4.407212	3.469484
N	-3.795280	4.959796	1.275988
C	-1.089015	5.053710	-1.643110
C	-0.027732	5.220044	-2.579991
C	0.120166	6.445945	-3.260939
C	-0.772357	7.493919	-2.993471
C	-1.806807	7.343458	-2.055842
C	-1.963806	6.122025	-1.381392
C	-2.538388	-1.362387	-3.964089
C	-1.417663	-1.976755	-4.598300
C	-1.554225	-2.533977	-5.886561
C	-2.794831	-2.477783	-6.536082
C	-3.905042	-1.876938	-5.922544
C	-3.768882	-1.323365	-4.640270
C	-1.008394	-3.980133	2.312351
C	0.318422	-4.419764	2.578000
C	0.526973	-5.700629	3.131438
C	-0.549133	-6.550502	3.410265
C	-1.858973	-6.135053	3.124995
C	-2.075061	-4.861924	2.582019
C	0.447701	2.400867	4.689584
C	-0.309430	3.276440	5.517780
C	0.233033	3.739280	6.736220
C	1.520294	3.342088	7.119962
C	2.280929	2.485719	6.309346
C	1.737692	2.020067	5.104014
C	1.765714	3.881388	-3.746263
C	2.361749	2.442753	-3.713147
C	3.813864	2.533135	-4.210953
C	1.517265	1.599973	-4.697050
C	2.330361	1.794869	-2.314382
C	1.003185	-2.569064	-4.190068
C	2.034660	-2.303839	-3.073514
C	3.533622	-4.219287	-2.401734
C	4.839236	-4.601958	-2.819305
C	5.469529	-5.687980	-2.184267
C	4.804245	-6.372795	-1.154336
C	3.482456	-5.980244	-0.761325
C	2.839813	-4.900409	-1.393434
C	4.314538	-2.890724	-4.020838
C	4.332256	-1.781876	-5.017159
C	5.477088	-7.532335	-0.460906
C	2.768783	-6.723711	0.340754
C	1.780479	-2.827713	1.268852
C	3.074118	-1.992937	1.444129
C	4.257967	-2.914392	1.809026
C	3.377244	-1.279979	0.118789
C	2.832445	-0.941639	2.550275
C	-2.532092	4.419254	5.701993
C	-3.837729	4.592212	4.902915
C	-4.010718	3.221287	2.772593
C	-4.047371	3.599710	1.402668
C	-4.338369	2.629655	0.429704
C	-4.554693	1.298139	0.821416
C	-4.433694	0.920227	2.200438
C	-4.173586	1.891840	3.184916
C	-3.632483	5.412734	2.505860
C	-3.305952	6.819899	2.872818
C	-4.954596	0.268771	-0.204973
C	-4.598555	-0.524342	2.598318
H	0.568031	4.647708	3.202908
H	-0.098582	5.687669	0.759315
H	-2.218381	3.769580	-3.666928
H	-2.746186	1.257981	-4.616084
H	-2.622628	-3.609347	-2.541006
H	-1.989952	-4.650588	-0.101225
H	-0.643437	-2.606542	4.589821
H	-0.047496	-0.102802	5.513444
H	0.932589	6.545675	-3.990754
H	-0.650087	8.447436	-3.529979
H	-2.499342	8.174482	-1.854228
H	-2.769890	5.963543	-0.644522
H	-0.678340	-3.003557	-6.350720
H	-2.891072	-2.915375	-7.541312
H	-4.875989	-1.841181	-6.438074
H	-4.628690	-0.851999	-4.140395
H	1.558457	-6.031616	3.326628
H	-0.360719	-7.545135	3.840961
H	-2.712218	-6.796455	3.335376
H	-3.098826	-4.513368	2.378657
H	-0.376253	4.399824	7.363985
H	1.931787	3.711921	8.071370
H	3.293291	2.180604	6.612546
H	2.315571	1.345635	4.454653
H	0.653724	3.349381	-2.122772
H	-0.276559	-1.567926	-2.953086
H	2.183677	-3.683363	3.078576
H	-1.840607	3.292658	4.140668
H	4.241427	1.518654	-4.343298
H	3.853174	3.070446	-5.176584
H	4.450994	3.085542	-3.490966
H	1.946881	0.581718	-4.802004
H	0.467757	1.499978	-4.350661
H	1.506891	2.068259	-5.700903
H	2.877248	0.829841	-2.336782
H	2.823200	2.429368	-1.549960
H	1.301667	1.559350	-1.962458
H	2.304914	-1.226633	-3.123100
H	1.578846	-2.457151	-2.071716
H	6.481440	-5.987696	-2.496401
H	1.828943	-4.600412	-1.083480
H	5.282382	-1.830037	-5.577208
H	3.483044	-1.872800	-5.724837
H	4.264257	-0.784309	-4.531511
H	5.581127	-7.359356	0.632164
H	4.897888	-8.474322	-0.571356
H	6.489697	-7.711705	-0.870130
H	2.666033	-7.806539	0.114222
H	3.322303	-6.663572	1.304014
H	1.753384	-6.317295	0.510795
H	5.195541	-2.323543	1.844319
H	4.145595	-3.385593	2.809002
H	4.386897	-3.719274	1.056706
H	4.260965	-0.622620	0.240227
H	3.597368	-2.009301	-0.683728
H	2.518012	-0.659015	-0.200065
H	3.736435	-0.310375	2.673726
H	1.981500	-0.282367	2.286594
H	2.601005	-1.403942	3.530713
H	-4.582899	3.882442	5.322161
H	-4.206456	5.607982	5.139018
H	-4.406186	2.918683	-0.629005
H	-4.094859	1.595569	4.242495
H	-2.349194	6.879945	3.432681
H	-3.211871	7.413478	1.946486
H	-4.091088	7.283117	3.507172
H	-5.981253	-0.110371	-0.011362
H	-4.937073	0.695137	-1.225696
H	-4.284407	-0.612861	-0.195824
H	-3.862414	-1.170012	2.075232
H	-4.452894	-0.663416	3.686456
H	-5.604779	-0.912673	2.333273

Conformation 15.
Multiplicity: 2
Charge: 0
E(B97-3c) = -5613.034887372199 Hartree
E(M06/def2-TZVP) = -5612.897545713929 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -5610.951484627647 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -5611.184342259526 Hartree
E(PBEh-3c) = -5604.838391608740 Hartree
E(PM6) = 188.52835 Kcal/mol
E(PM7) = 51.88305 Kcal/mol
E(ωB97X-V/def2-TZVP) = -5614.592697511664 Hartree
E(GFN1-xTB) = -265.552589281974 Hartree
E(GFN2-xTB) = -259.283545067739 Hartree
E(GFN-FF) = -33.836955993219 Hartree

Coordinates:

Cu	1.352590	1.461207	0.287010
N	2.484604	0.789626	-1.264748
N	0.314708	2.640160	-0.997144
N	0.262403	2.179056	1.846835
N	2.344701	0.233238	1.560983
C	3.524448	-0.117356	-1.191216
C	2.354917	1.119915	-2.599933
C	0.473872	2.724287	-2.368121
C	-0.663037	3.559289	-0.665550
C	-0.705603	3.163800	1.790220
C	0.332980	1.783765	3.168716
C	2.134529	0.093151	2.920622
C	3.404267	-0.596856	1.247298
C	4.072518	-0.355755	-2.512564
C	3.336019	0.399607	-3.387882
C	-0.439070	3.710129	-2.914190
C	-1.147260	4.223904	-1.859256
C	-1.254585	3.400070	3.111383
C	-0.620545	2.533371	3.963315
C	3.075906	-0.862255	3.472675
C	3.858665	-1.294527	2.434075
C	1.406528	2.005754	-3.145155
C	-1.144500	3.832239	0.629493
C	1.185682	0.794552	3.693670
C	3.981765	-0.766098	-0.026268
O	-2.534567	2.394312	-5.597952
O	-6.116710	2.967987	1.388366
O	1.523770	-3.514625	5.380324
O	3.762986	-5.517348	-1.885151
N	-0.799670	1.157068	-4.756326
N	-3.825021	3.109958	1.080282
N	-3.819860	0.553233	2.433066
N	-1.999927	-0.374382	3.385485
N	0.263337	-1.743283	4.658353
N	3.630655	-3.324436	-1.147900
N	1.390194	-3.178728	-2.957737
N	0.526649	-1.228761	-3.686447
C	1.386843	2.227724	-4.621998
C	0.241882	1.870346	-5.384904
C	0.180707	2.203650	-6.753861
C	1.260709	2.844556	-7.373659
C	2.415298	3.159308	-6.638279
C	2.469052	2.856472	-5.271332
C	-2.213171	4.873081	0.768607
C	-3.566911	4.487430	0.976150
C	-4.579251	5.465130	1.066581
C	-4.241075	6.820617	0.960136
C	-2.909432	7.216775	0.762527
C	-1.906521	6.241088	0.665670
C	1.121351	0.485838	5.153836
C	0.737575	-0.807081	5.601152
C	0.809663	-1.123405	6.973481
C	1.216445	-0.156476	7.901258
C	1.553332	1.138306	7.473291
C	1.510317	1.448863	6.107851
C	5.128040	-1.723967	-0.146682
C	4.926228	-3.020997	-0.696193
C	5.994855	-3.938596	-0.766558
C	7.260987	-3.560326	-0.301008
C	7.477729	-2.281884	0.235640
C	6.410542	-1.374915	0.311113
C	-2.136027	1.477154	-4.881722
C	-3.099002	0.611523	-4.025377
C	-2.942434	-0.874360	-4.410070
C	-4.534119	1.080097	-4.298254
C	-2.767260	0.808712	-2.530357
C	-5.006943	2.451985	1.306947
C	-4.814753	0.925183	1.446112
C	-3.975961	0.716320	3.808495
C	-2.827730	0.118747	4.389083
C	-2.672160	0.133470	5.786169
C	-3.654694	0.749558	6.577289
C	-4.810449	1.347641	5.972311
C	-4.974618	1.329671	4.575723
C	-2.603572	-0.092096	2.238542
C	-2.035535	-0.371546	0.892436
C	-3.485138	0.789426	8.075749
C	-5.852018	2.011368	6.836616
C	0.707292	-3.047780	4.587540
C	0.124539	-3.874111	3.410201
C	0.542745	-3.220636	2.076294
C	0.702089	-5.293449	3.489032
C	-1.413550	-3.922108	3.518153
C	3.142024	-4.473369	-1.716116
C	1.659446	-4.338802	-2.131230
C	1.803013	-3.042525	-4.281931
C	1.241696	-1.817164	-4.724946
C	1.487520	-1.378691	-6.037857
C	2.293116	-2.160869	-6.880401
C	2.852876	-3.397500	-6.414664
C	2.605357	-3.843835	-5.104346
C	0.642907	-2.047157	-2.649228
C	0.088320	-1.783194	-1.294225
C	2.578274	-1.689380	-8.284680
C	3.719922	-4.221226	-7.332389
H	4.907214	-1.029620	-2.733510
H	3.429798	0.454462	-4.476468
H	-0.532553	3.966961	-3.974418
H	-1.929557	4.989517	-1.877598
H	-2.034191	4.132926	3.345656
H	-0.791184	2.393996	5.034863
H	3.121803	-1.172462	4.521746
H	4.678343	-2.019784	2.459906
H	-0.725413	1.950549	-7.318585
H	1.201057	3.095667	-8.443596
H	3.266307	3.659271	-7.124209
H	3.350865	3.136723	-4.675684
H	-5.615389	5.138760	1.215009
H	-5.036948	7.577283	1.032174
H	-2.650263	8.282595	0.680780
H	-0.857703	6.532160	0.504824
H	0.541491	-2.137386	7.296190
H	1.264994	-0.415961	8.969746
H	1.869509	1.900905	8.200480
H	1.810704	2.447394	5.756341
H	5.805562	-4.935356	-1.182270
H	8.089813	-4.281951	-0.359724
H	8.474405	-1.990457	0.598321
H	6.559880	-0.370813	0.735413
H	-0.484241	0.378974	-4.137907
H	-2.976096	2.535142	1.080205
H	-0.422882	-1.363666	3.970761
H	2.989843	-2.524977	-1.117553
H	-3.665580	-1.492535	-3.837679
H	-3.146609	-1.027721	-5.488983
H	-1.923808	-1.253785	-4.196087
H	-5.250025	0.489927	-3.690381
H	-4.654691	2.152355	-4.052004
H	-4.795261	0.960172	-5.367266
H	-3.457323	0.197924	-1.909903
H	-1.731649	0.496251	-2.292799
H	-2.873557	1.870113	-2.228084
H	-5.803478	0.509671	1.722590
H	-4.524138	0.498790	0.464782
H	-1.783829	-0.315593	6.252432
H	-5.850797	1.804253	4.108449
H	-1.068290	-0.880872	1.033569
H	-2.690151	-1.016390	0.270906
H	-1.837016	0.560028	0.321110
H	-3.474513	1.831265	8.460802
H	-4.317548	0.273041	8.599693
H	-2.537548	0.307366	8.383220
H	-6.285758	1.303525	7.574558
H	-5.421994	2.848577	7.426711
H	-6.682209	2.418873	6.229011
H	0.129391	-3.804421	1.226266
H	0.167405	-2.181994	1.990883
H	1.645899	-3.184379	1.971544
H	0.315257	-5.909595	2.651790
H	1.807544	-5.275440	3.438855
H	0.427180	-5.781469	4.443757
H	-1.830750	-4.550229	2.703211
H	-1.727666	-4.369407	4.482838
H	-1.871496	-2.915821	3.441816
H	1.400650	-5.266563	-2.677618
H	1.027171	-4.288059	-1.221634
H	1.067395	-0.428110	-6.395363
H	3.050590	-4.781573	-4.738608
H	0.877763	-1.751415	-0.514089
H	-0.392626	-0.791185	-1.311565
H	-0.661806	-2.539569	-0.983403
H	2.209835	-2.410718	-9.045012
H	2.100466	-0.710992	-8.482966
H	3.668134	-1.576384	-8.466726
H	4.612329	-3.653595	-7.672002

H	4.074796	-5.143722	-6.834930
H	3.174435	-4.519304	-8.252934

Conformation 27.
Multiplicity: 2
Charge: 0
E(B97-3c) = -5613.042555915213 Hartree
E(M06/def2-TZVP) = -5612.901562009599 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -5610.956789533199 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -5611.191183441710 Hartree
E(PBEh-3c) = -5604.839522715391 Hartree
E(PM6) = 174.80311 Kcal/mol
E(PM7) = 47.79992 Kcal/mol
E(ωB97X-V/def2-TZVP) = -5614.598870664975 Hartree
E(GFN1-xTB) = -265.559776830230 Hartree
E(GFN2-xTB) = -259.287281656695 Hartree
E(GFN-FF) = -33.850614778996 Hartree

Coordinates:

Cu	1.047128	-0.274766	-0.178021
N	2.034567	1.410012	0.366673
N	1.394981	0.156118	-2.130589
N	0.029503	-1.934061	-0.723305
N	0.532691	-0.599190	1.758905
C	2.183092	1.911720	1.642266
C	2.797590	2.214496	-0.457116
C	2.119358	1.218265	-2.627270
C	0.898422	-0.519652	-3.225816
C	-0.113023	-2.429072	-2.002726
C	-0.495590	-2.888894	0.121926
C	-0.231414	-1.636203	2.250098
C	0.756885	0.253548	2.821899
C	3.078774	3.051908	1.629767
C	3.481633	3.222907	0.328438
C	2.054795	1.233180	-4.076102
C	1.286987	0.158179	-4.448808
C	-0.683813	-3.761791	-1.960771
C	-0.912214	-4.051289	-0.639894
C	-0.512533	-1.423675	3.658081
C	0.098218	-0.247896	4.012529
C	2.835307	2.159954	-1.863853
C	0.198777	-1.742322	-3.191047
C	-0.694848	-2.741997	1.510211
C	1.532894	1.427224	2.795409
O	1.630978	7.068090	-2.462834
O	3.188315	-4.616261	-6.145886
O	-4.870137	-4.748301	-0.014543
O	-1.867772	5.011926	3.563373
N	1.906269	4.812774	-2.097165
N	2.074721	-3.174103	-4.712684
N	4.431288	-2.592671	-3.371808
N	4.882959	-0.534660	-2.549535
N	-3.477060	-3.181178	0.922517
N	-0.604676	3.094003	3.265316
N	-2.811604	1.939257	2.007846
N	-2.895327	-0.239304	1.431934
C	3.632772	3.196073	-2.589414
C	3.139942	4.527745	-2.704328
C	3.895378	5.489698	-3.409716
C	5.122883	5.125460	-3.980109
C	5.618180	3.817049	-3.861512
C	4.868786	2.855497	-3.167181
C	-0.189765	-2.383888	-4.486549
C	0.770240	-3.122622	-5.231181
C	0.393560	-3.768281	-6.427924
C	-0.928905	-3.667898	-6.880207
C	-1.884205	-2.935496	-6.158827
C	-1.508767	-2.301530	-4.965279
C	-1.489333	-3.788642	2.214347
C	-2.855098	-4.013895	1.873082
C	-3.563503	-5.052347	2.519020
C	-2.939923	-5.835951	3.497532
C	-1.603455	-5.601582	3.858112
C	-0.891450	-4.581229	3.215574
C	1.548369	2.311633	4.002766
C	0.461632	3.216602	4.172648
C	0.482791	4.166036	5.213372
C	1.567836	4.188038	6.100841
C	2.628471	3.278513	5.966105
C	2.615318	2.348736	4.914148
C	1.240760	6.016006	-1.964623
C	-0.051735	5.924513	-1.102949
C	-0.701914	7.314375	-1.081178
C	0.322308	5.501354	0.335917
C	-1.028950	4.901753	-1.720535
C	3.159757	-3.878743	-5.166508
C	4.422345	-3.703046	-4.298491
C	4.087883	-2.630837	-2.018684
C	4.397300	-1.334871	-1.523212
C	4.200045	-1.056533	-0.158546
C	3.689443	-2.056987	0.686488
C	3.334123	-3.342310	0.155262
C	3.539358	-3.631658	-1.205482
C	4.889061	-1.295654	-3.629555
C	5.295858	-0.861972	-4.996555
C	3.560382	-1.800354	2.167101
C	2.748204	-4.393755	1.062253
C	-4.437230	-3.598228	0.013168
C	-4.940022	-2.503692	-0.964769
C	-5.855384	-3.176425	-1.996935
C	-5.738677	-1.455334	-0.159689
C	-3.751128	-1.837212	-1.685791
C	-1.665776	3.926443	3.029058
C	-2.622947	3.373691	1.947387
C	-3.387509	1.273794	3.089218
C	-3.435204	-0.089792	2.706008
C	-3.958154	-1.041034	3.599443
C	-4.407797	-0.621202	4.860993
C	-4.344878	0.762531	5.234754
C	-3.832735	1.719328	4.340383
C	-2.527609	0.973364	1.040317
C	-1.867646	1.304174	-0.255036
C	-4.957680	-1.636915	5.831252
C	-4.830566	1.195558	6.594514
H	3.361845	3.635652	2.511781
H	4.163704	3.975152	-0.082111
H	2.539110	1.981417	-4.712160
H	1.003480	-0.162542	-5.457465
H	-0.885579	-4.383683	-2.839474
H	-1.345255	-4.960581	-0.209629
H	-1.120663	-2.084758	4.282348
H	0.111528	0.246129	4.990156
H	3.498966	6.508425	-3.491546
H	5.701802	5.886618	-4.525511
H	6.588104	3.545379	-4.304603
H	5.219133	1.817894	-3.036277
H	1.148669	-4.345128	-6.974899
H	-1.213762	-4.175413	-7.814309
H	-2.920598	-2.860800	-6.519523
H	-2.244986	-1.729951	-4.381151
H	-4.604341	-5.237268	2.230115
H	-3.512000	-6.638332	3.987852
H	-1.114306	-6.216882	4.627614
H	0.162796	-4.394511	3.470537
H	-0.348453	4.876451	5.298999
H	1.579368	4.930396	6.913185
H	3.471636	3.298952	6.672172
H	3.449923	1.644477	4.778415
H	1.489555	4.011742	-1.616709
H	2.221926	-2.609250	-3.868209
H	-3.132534	-2.202539	0.868823
H	-0.586650	2.225387	2.719702
H	-1.631439	7.290401	-0.477399
H	-0.015925	8.064927	-0.644798
H	-0.949295	7.654886	-2.104919
H	-0.553691	5.607715	1.008624
H	0.676728	4.451579	0.397623
H	1.125976	6.144437	0.746874
H	-1.972657	4.879098	-1.135419
H	-1.289461	5.171012	-2.763784
H	-0.619893	3.869841	-1.731590
H	4.570706	-4.646944	-3.733566
H	5.273849	-3.625030	-5.001726
H	4.468447	-0.068356	0.241516
H	3.263927	-4.619415	-1.605993
H	5.566366	0.208122	-4.965852
H	6.167319	-1.435692	-5.376784
H	4.467484	-0.992889	-5.723935
H	2.555642	-2.064385	2.551172
H	4.291686	-2.410038	2.741009
H	3.742527	-0.735891	2.408389
H	3.441686	-4.658312	1.888560
H	1.810388	-4.036629	1.536714
H	2.508276	-5.320560	0.507421
H	-6.257762	-2.417269	-2.698039
H	-5.304918	-3.939474	-2.581387
H	-6.701403	-3.691328	-1.503586
H	-6.157005	-0.690386	-0.846719
H	-6.584897	-1.929411	0.377599
H	-5.101320	-0.935721	0.580451
H	-4.120690	-1.066783	-2.394555
H	-3.059004	-1.337361	-0.981094
H	-3.167406	-2.583597	-2.258794
H	-3.585798	3.907036	2.078836
H	-2.220893	3.644231	0.950321
H	-4.006010	-2.102455	3.319330
H	-3.779412	2.779950	4.629665
H	-0.905752	1.837403	-0.101362
H	-1.650588	0.364786	-0.793807
H	-2.505781	1.942347	-0.901684
H	-6.011169	-1.416270	6.106085

H	-4.924755	-2.657259	5.403945
H	-4.385096	-1.649311	6.783086
H	-4.275290	0.685356	7.410057
H	-4.715336	2.286747	6.737985
H	-5.901933	0.944138	6.745692

Conformation 3.
Multiplicity: 2
Charge: 0
E(B97-3c) = -5613.028293440165 Hartree
E(M06/def2-TZVP) = -5612.884558904302 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -5610.944305474064 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -5611.177832988753 Hartree
E(PBEh-3c) = -5604.825993825991 Hartree
E(PM6) = 180.56968 Kcal/mol
E(PM7) = 63.92277 Kcal/mol
E(ωB97X-V/def2-TZVP) = -5614.582834209616 Hartree
E(GFN1-xTB) = -265.538406165897 Hartree
E(GFN2-xTB) = -259.267604748224 Hartree
E(GFN-FF) = -33.827463137018 Hartree

Coordinates:

Cu	-0.760790	-0.044570	-1.390913
N	0.825794	-1.294839	-1.188298
N	0.489014	1.551391	-1.425073
N	-2.350265	1.214471	-1.548919
N	-2.021806	-1.618510	-1.170337
C	0.790672	-2.667775	-1.060933
C	2.159424	-0.945113	-1.224912
C	1.864713	1.517848	-1.350157
C	0.138791	2.882405	-1.515496
C	-2.316667	2.582146	-1.731432
C	-3.683943	0.861858	-1.542677
C	-3.400105	-1.572888	-1.130785
C	-1.676761	-2.939171	-0.969208
C	2.138454	-3.203093	-1.025759
C	2.989380	-2.131801	-1.131742
C	2.399641	2.866269	-1.366107
C	1.326456	3.715508	-1.456900
C	-3.663002	3.097042	-1.899307
C	-4.514054	2.030614	-1.758861
C	-3.939766	-2.896383	-0.882078
C	-2.868027	-3.747124	-0.787240
C	2.668945	0.364110	-1.286203
C	-1.164473	3.389857	-1.694480
C	-4.199649	-0.426516	-1.299270
C	-0.369012	-3.457977	-0.931750
O	5.311709	1.661100	2.833676
O	0.164607	6.091374	-5.817234
O	-6.012909	-0.205363	3.367896
O	0.060237	-5.316618	3.758556
N	3.891340	1.184609	1.089578
N	-0.330461	4.645553	-4.073913
N	0.976999	2.546880	-5.378660
N	2.135330	0.819205	-4.483879
N	-4.985413	-0.238113	1.307498
N	-0.107141	-4.253189	1.706020
N	0.859617	-2.688371	4.722387
N	1.848556	-2.469284	6.742625
C	4.150299	0.549178	-1.219668
C	4.750130	0.957650	0.005710
C	6.150595	1.125698	0.071418
C	6.931435	0.887201	-1.067956
C	6.345238	0.484119	-2.278823
C	4.953394	0.318210	-2.349728
C	-1.326498	4.864055	-1.882644
C	-0.905806	5.476453	-3.097523
C	-1.079388	6.864476	-3.283846
C	-1.662270	7.633708	-2.268226
C	-2.079073	7.042902	-1.065580
C	-1.910147	5.663023	-0.883041
C	-5.658077	-0.546070	-0.980432
C	-6.029026	-0.441281	0.393647
C	-7.384769	-0.545474	0.766085
C	-8.356840	-0.748170	-0.223816
C	-8.002947	-0.850056	-1.578442
C	-6.652173	-0.749107	-1.949258
C	-0.202341	-4.910348	-0.607158
C	-0.080983	-5.290361	0.759740
C	0.059476	-6.649220	1.108029
C	0.079757	-7.619126	0.096289
C	-0.037311	-7.257459	-1.254954
C	-0.179010	-5.903974	-1.598698
C	4.169036	1.555296	2.389802
C	2.912227	1.925597	3.224624
C	3.214219	1.622889	4.700229
C	1.641281	1.168496	2.788572
C	2.705758	3.445153	3.021455
C	0.166492	4.975377	-5.308930
C	0.738673	3.780438	-6.097999
C	0.052226	1.521032	-5.174270
C	0.805770	0.445480	-4.629887
C	0.158424	-0.771984	-4.350270
C	-1.221123	-0.895339	-4.591454
C	-1.974343	0.223676	-5.080049
C	-1.330749	1.436337	-5.385259
C	2.211886	2.061506	-4.927363
C	3.441178	2.904705	-4.932833
C	-1.910403	-2.219169	-4.376250
C	-3.464661	0.099741	-5.267950
C	-4.996432	-0.141808	2.680740
C	-3.596456	0.091272	3.322648
C	-3.606124	1.534245	3.871107
C	-3.465850	-0.908126	4.487282
C	-2.415489	-0.084851	2.348751
C	-0.046969	-4.302792	3.080133
C	-0.150686	-2.903834	3.722150
C	2.194313	-2.400376	4.462776
C	2.788814	-2.245178	5.745706
C	4.149966	-1.901053	5.829527
C	4.899146	-1.736038	4.652707
C	4.292000	-1.944826	3.370337
C	2.925768	-2.271548	3.273500
C	0.720854	-2.740369	6.111633
C	-0.573054	-3.098818	6.761627
C	6.344016	-1.311018	4.728059
C	5.129200	-1.840149	2.122320
H	2.385812	-4.265933	-0.931033
H	4.083912	-2.129231	-1.150368
H	3.464658	3.116132	-1.313975
H	1.324558	4.810525	-1.486918
H	-3.912248	4.147095	-2.083286
H	-5.608239	2.017335	-1.802153
H	-5.007356	-3.128506	-0.804861
H	-2.866467	-4.828713	-0.614908
H	6.595813	1.437699	1.023691
H	8.022160	1.020191	-1.002599
H	6.968677	0.299804	-3.166348
H	4.449831	0.021639	-3.283286
H	-0.754919	7.311173	-4.231118
H	-1.791350	8.715329	-2.425035
H	-2.533145	7.652598	-0.270723
H	-2.229584	5.180583	0.052998
H	-7.644211	-0.465233	1.828912
H	-9.413255	-0.828007	0.074626
H	-8.774515	-1.009900	-2.345830
H	-6.353658	-0.829914	-3.005735
H	0.150892	-6.914924	2.168300
H	0.190856	-8.678083	0.374464
H	-0.018955	-8.026190	-2.041364
H	-0.275552	-5.600497	-2.652221
H	2.899637	1.076032	0.867293
H	-0.237407	3.660170	-3.803397
H	-4.065061	-0.169680	0.868461
H	-0.183160	-3.319729	1.291435
H	2.389322	1.990262	5.343201
H	3.332652	0.534869	4.868501
H	4.155307	2.116075	5.007208
H	0.808136	1.425704	3.474410
H	1.291779	1.443116	1.768560
H	1.792024	0.071346	2.837768
H	1.851474	3.797659	3.635397
H	3.609457	4.007363	3.329206
H	2.489138	3.686266	1.959996
H	0.040291	3.584222	-6.939593
H	1.681051	4.137360	-6.554524
H	0.737789	-1.623507	-3.965969
H	-1.912730	2.289780	-5.766028
H	4.256331	2.344252	-4.441866
H	3.766236	3.170639	-5.961111
H	3.281147	3.850606	-4.375125
H	-2.795512	-2.127420	-3.715952
H	-2.274168	-2.640863	-5.338008
H	-1.226786	-2.958743	-3.918782
H	-3.726575	-0.701987	-5.990502
H	-3.965674	-0.160613	-4.311219
H	-3.907700	1.045800	-5.632877
H	-2.670740	1.742031	4.430387
H	-3.686445	2.273606	3.047859
H	-4.466148	1.680542	4.552901
H	-2.537881	-0.710176	5.062043
H	-4.334519	-0.820274	5.166791
H	-3.433403	-1.953737	4.116358
H	-1.458431	0.064550	2.889319
H	-2.388419	-1.100520	1.901095
H	-2.422952	0.658717	1.523264
H	-0.092623	-2.096649	2.959649
H	-1.148962	-2.825402	4.196028
H	4.615968	-1.755830	6.815663
H	2.470676	-2.442684	2.284745
H	-0.921612	-4.096518	6.423239
H	-0.417085	-3.122340	7.854300

H	-1.376861	-2.364721	6.539185
H	6.485859	-0.323164	4.238969
H	6.682155	-1.224539	5.778315
H	7.018213	-2.026193	4.211204
H	5.908666	-2.632064	2.092984
H	4.510066	-1.941886	1.211579
H	5.665752	-0.872230	2.066399

Conformation 31.
Multiplicity: 2
Charge: 0
E(B97-3c) = -5613.001675257173 Hartree
E(M06/def2-TZVP) = -5612.861948446687 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -5610.919969589283 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -5611.152113263775 Hartree
E(PBEh-3c) = -5604.804784540860 Hartree
E(PM6) = 197.04998 Kcal/mol
E(PM7) = 82.38588 Kcal/mol
E(ωB97X-V/def2-TZVP) = -5614.557622015721 Hartree
E(GFN1-xTB) = -265.517724803432 Hartree
E(GFN2-xTB) = -259.253122296361 Hartree
E(GFN-FF) = -33.801568872292 Hartree

Coordinates:

Cu	0.130463	0.077038	0.057900
N	-0.358028	-1.803844	0.637650
N	-1.206353	0.835531	1.383997
N	0.594545	1.958151	-0.539991
N	1.508623	-0.670043	-1.227446
C	0.155862	-2.985892	0.142065
C	-1.347596	-2.160529	1.533439
C	-2.047568	0.122788	2.215896
C	-1.420011	2.169402	1.673269
C	0.145663	3.142656	0.009162
C	1.437312	2.306665	-1.574275
C	2.237152	0.031410	-2.162469
C	1.813916	-2.002524	-1.425823
C	-0.531036	-4.116920	0.734504
C	-1.459636	-3.604225	1.604831
C	-2.816535	1.031058	3.044890
C	-2.421039	2.302615	2.713590
C	0.742309	4.269929	-0.679477
C	1.527117	3.749912	-1.677891
C	3.053141	-0.875023	-2.946708
C	2.808339	-2.136518	-2.474081
C	-2.139560	-1.279745	2.297911
C	-0.780737	3.266300	1.061912
C	2.167460	1.418496	-2.385349
C	1.178949	-3.103845	-0.819445
O	-0.801050	-3.021974	6.860105
O	1.541378	5.227627	5.118347
O	0.217441	0.339519	-4.147884
O	-0.359729	-4.928083	-5.309963
N	-1.135072	-2.296574	4.702912
N	0.575919	4.121524	3.324996
N	2.314868	2.567250	5.995803
N	3.056833	2.232583	8.104391
N	0.667933	2.530934	-4.643208
N	0.209938	-3.889435	-3.319753
N	-1.628119	-2.575465	-6.223865
N	-2.808380	-2.912795	-8.125434
C	-3.062554	-1.874202	3.315428
C	-2.521730	-2.386718	4.530988
C	-3.384672	-2.954974	5.493722
C	-4.763613	-3.001332	5.251219
C	-5.306432	-2.490513	4.061928
C	-4.450349	-1.931330	3.101687
C	-1.041393	4.633012	1.615421
C	-0.323336	5.048191	2.773398
C	-0.530473	6.334384	3.312794
C	-1.447132	7.198672	2.698871
C	-2.161327	6.802105	1.557355
C	-1.953395	5.521296	1.022430
C	2.847114	1.983199	-3.585055
C	2.083770	2.522748	-4.656282
C	2.742542	3.126186	-5.746859
C	4.139834	3.187945	-5.797817
C	4.901594	2.632100	-4.758379
C	4.253415	2.038946	-3.667065
C	1.493776	-4.466206	-1.352884
C	0.979657	-4.840360	-2.630326
C	1.248457	-6.125458	-3.146952
C	2.015137	-7.027443	-2.397130
C	2.522181	-6.672236	-1.137555
C	2.257007	-5.393902	-0.624113
C	-0.346681	-2.623407	5.788515
C	1.178152	-2.535181	5.510493
C	1.886907	-2.211921	6.834536
C	1.545277	-1.476100	4.451146
C	1.594822	-3.937449	5.006591
C	1.425974	4.242067	4.400364
C	2.283065	2.976507	4.617700
C	1.304362	1.870627	6.648360
C	1.803696	1.651458	7.962256
C	1.024749	0.916823	8.874447
C	-0.235087	0.435389	8.482067
C	-0.743147	0.716721	7.171054
C	0.036884	1.430740	6.241538
C	3.330344	2.775606	6.932592
C	4.554337	3.562599	6.604720
C	-1.053407	-0.407232	9.427683
C	-2.129948	0.264793	6.795996
C	-0.187571	1.479090	-4.375557
C	-1.685087	1.868297	-4.332315
C	-2.067153	2.759289	-5.532147
C	-2.526253	0.584321	-4.369967
C	-1.928502	2.612549	-2.998358
C	-0.400439	-3.965715	-4.553482
C	-1.222361	-2.693601	-4.849936
C	-1.041286	-1.762012	-7.188387
C	-1.808089	-1.982716	-8.366864
C	-1.483469	-1.273112	-9.537520
C	-0.412190	-0.365483	-9.525745
C	0.352743	-0.165627	-8.329826
C	0.038447	-0.869771	-7.153200
C	-2.675281	-3.251083	-6.855095
C	-3.521110	-4.244548	-6.133545
C	-0.055562	0.397450	-10.778255
C	1.513278	0.798514	-8.328242
H	-0.321843	-5.165979	0.500909
H	-2.174008	-4.142864	2.236662
H	-3.569034	0.720452	3.776789
H	-2.776127	3.255745	3.120214
H	0.568181	5.320321	-0.423061
H	2.146207	4.286690	-2.404786
H	3.715889	-0.578489	-3.765187
H	3.235718	-3.086568	-2.811875
H	-2.947365	-3.341488	6.421899
H	-5.424064	-3.446059	6.011111
H	-6.390348	-2.529227	3.879435
H	-4.853820	-1.532352	2.158689
H	0.035464	6.628265	4.205247
H	-1.605027	8.200426	3.126285
H	-2.880740	7.486582	1.084274
H	-2.503790	5.190858	0.128437
H	2.138522	3.533317	-6.571885
H	4.633792	3.661804	-6.659016
H	6.000316	2.671281	-4.790763
H	4.840034	1.628351	-2.831673
H	0.845291	-6.387725	-4.132544
H	2.218028	-8.027073	-2.810443
H	3.125047	-7.385523	-0.556617
H	2.647950	-5.095089	0.360300
H	-0.634479	-1.918701	3.895860
H	0.587879	3.220751	2.837575
H	0.228207	3.384568	-4.990787
H	0.120887	-2.992053	-2.833357
H	2.986193	-2.266253	6.703048
H	1.626434	-1.196026	7.190378
H	1.583240	-2.930449	7.618553
H	2.648647	-1.410192	4.364518
H	1.173919	-1.725670	3.432617
H	1.168897	-0.473951	4.739199
H	2.690237	-3.969709	4.833407
H	1.338567	-4.713887	5.754280
H	1.087032	-4.191070	4.052679
H	1.929274	2.128151	3.991129
H	3.314225	3.216223	4.289438
H	1.411869	0.715955	9.884593
H	-0.366498	1.652508	5.240388
H	5.174407	3.634414	7.515381
H	5.162145	3.086038	5.805859
H	4.285165	4.584471	6.266020
H	-2.060289	0.024137	9.610333
H	-1.209446	-1.423105	9.004917
H	-0.548636	-0.516930	10.406442
H	-2.270448	-0.819854	6.972224
H	-2.902623	0.784725	7.402810
H	-2.342906	0.467547	5.730276
H	-3.161303	2.937238	-5.532252
H	-1.593376	3.764139	-5.496258
H	-1.800771	2.275906	-6.494084
H	-3.601178	0.837587	-4.280022
H	-2.376532	0.033234	-5.319096
H	-2.253076	-0.085752	-3.533348
H	-2.996372	2.900658	-2.913820
H	-1.673368	1.966454	-2.134992
H	-1.312111	3.530179	-2.915923
H	-2.122049	-2.722425	-4.196452
H	-0.658530	-1.781950	-4.557724
H	-2.072106	-1.436319	-10.452985
H	0.627285	-0.711325	-6.238271

H	-4.037504	-3.796516	-5.257598
H	-4.285710	-4.624637	-6.833528
H	-2.904287	-5.091287	-5.769179
H	0.981806	0.181794	-11.113718
H	-0.736970	0.141113	-11.611963
H	-0.108797	1.497170	-10.625692
H	1.196288	1.830474	-8.596017
H	2.000948	0.841943	-7.335671
H	2.288336	0.515079	-9.072534

Conformation 32.
Multiplicity: 2
Charge: 0
E(B97-3c) = -5613.012411494140 Hartree
E(M06/def2-TZVP) = -5612.873146275971 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -5610.925860426999 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -5611.159603419211 Hartree
E(PBEh-3c) = -5604.808512107461 Hartree
E(PM6) = 209.68398 Kcal/mol
E(PM7) = 71.95218 Kcal/mol
E(ωB97X-V/def2-TZVP) = -5614.570210628630 Hartree
E(GFN1-xTB) = -265.536137349420 Hartree
E(GFN2-xTB) = -259.265178967879 Hartree
E(GFN-FF) = -33.811077111268 Hartree

Coordinates:

Cu	-0.004864	1.349080	0.403652
N	-0.203351	1.130173	2.404906
N	1.297212	-0.209530	0.339172
N	0.160037	1.548063	-1.601024
N	-1.427627	2.805019	0.436943
C	-1.066606	1.809337	3.240751
C	0.504660	0.260614	3.204649
C	1.786564	-0.907150	1.424193
C	1.806012	-0.834732	-0.782135
C	0.909891	0.768049	-2.450868
C	-0.464521	2.482938	-2.395815
C	-1.919447	3.490546	-0.652919
C	-2.119289	3.275977	1.534427
C	-0.908262	1.340433	4.605940
C	0.078548	0.388299	4.584408
C	2.631799	-1.997229	0.975757
C	2.625863	-1.969358	-0.395943
C	0.845012	1.295409	-3.802601
C	-0.020180	2.355611	-3.769025
C	-2.945377	4.423798	-0.236210
C	-3.056808	4.305088	1.127600
C	1.460591	-0.677885	2.772912
C	1.597129	-0.413909	-2.109087
C	-1.500469	3.336653	-1.986164
C	-1.968164	2.822791	2.860117
O	-0.924530	-4.551480	4.919844
O	-2.260147	-2.772449	-3.970041
O	-2.354474	0.568037	-3.337433
O	-0.249586	6.063360	6.413971
N	0.046371	-2.895102	3.651675
N	-0.175762	-1.849751	-3.935101
N	0.751952	-4.705444	-3.600440
N	2.381618	-4.803342	-2.036500
N	-3.937759	2.048710	-2.604366
N	-0.759098	4.541704	4.740648
N	1.967433	4.098292	4.263012
N	2.995340	2.174181	3.654756
C	2.052638	-1.576540	3.811672
C	1.301288	-2.704442	4.248988
C	1.827884	-3.550459	5.247585
C	3.086998	-3.267642	5.796114
C	3.830801	-2.154352	5.372548
C	3.307811	-1.308628	4.381042
C	2.122679	-1.206309	-3.258660
C	1.224635	-1.815826	-4.184544
C	1.739441	-2.372542	-5.370438
C	3.118698	-2.418391	-5.610140
C	4.008809	-1.884638	-4.669819
C	3.504968	-1.266552	-3.516131
C	-2.369744	3.900024	-3.061707
C	-3.565944	3.195520	-3.368913
C	-4.419975	3.671913	-4.377313
C	-4.099205	4.838763	-5.086686
C	-2.915655	5.532980	-4.794268
C	-2.056965	5.062060	-3.788623
C	-2.777821	3.486209	3.927312
C	-2.149750	4.368731	4.852626
C	-2.921565	5.027491	5.833613
C	-4.302562	4.800613	5.899359
C	-4.932130	3.926060	5.000557
C	-4.165574	3.278233	4.021239
C	-0.997613	-3.721110	4.018362
C	-2.280887	-3.505223	3.164777
C	-3.391204	-4.386824	3.751407
C	-1.987532	-3.926133	1.708450
C	-2.713231	-2.021961	3.200999
C	-1.042204	-2.916968	-4.040539
C	-0.511247	-4.361398	-4.212135
C	1.877878	-5.202799	-4.248343
C	2.891820	-5.232074	-3.252240
C	4.190666	-5.639168	-3.603913
C	4.464197	-6.018067	-4.927457
C	3.422390	-6.008344	-5.913015
C	2.121376	-5.603078	-5.567895
C	1.113307	-4.501519	-2.267444
C	0.144526	-4.003189	-1.250501
C	5.857084	-6.448250	-5.316946
C	3.723732	-6.432754	-7.328657
C	-3.258162	0.847791	-2.550493
C	-3.746772	-0.145905	-1.463973
C	-4.516926	0.532220	-0.315392
C	-4.639128	-1.181750	-2.182203
C	-2.505036	-0.846010	-0.882617
C	0.081595	5.311450	5.502785
C	1.569323	5.202220	5.110336
C	2.017091	4.106296	2.867263
C	2.677073	2.898020	2.513480
C	2.925907	2.622609	1.157627
C	2.514833	3.541392	0.176892
C	1.796205	4.725567	0.550421
C	1.552677	5.013706	1.905728
C	2.566692	2.898641	4.672375
C	2.658917	2.510205	6.108373
C	2.881937	3.311326	-1.267343
C	1.294738	5.665870	-0.516074
H	-1.490214	1.698663	5.462174
H	0.484805	-0.194804	5.417442
H	3.136054	-2.709022	1.638046
H	3.088991	-2.689303	-1.080678
H	1.387479	0.891251	-4.663308
H	-0.357226	2.984331	-4.598690
H	-3.482193	5.103166	-0.907758
H	-3.709026	4.861625	1.808391
H	1.229715	-4.407214	5.579974
H	3.490154	-3.933969	6.574197
H	4.814741	-1.940429	5.816081
H	3.841565	-0.405108	4.048004
H	1.038956	-2.781257	-6.112167
H	3.493244	-2.885825	-6.532010
H	5.093908	-1.926657	-4.843325
H	4.189508	-0.796575	-2.794274
H	-5.337173	3.108292	-4.603756
H	-4.774581	5.202485	-5.875515
H	-2.659445	6.447968	-5.349129
H	-1.130709	5.605908	-3.548101
H	-2.415745	5.711696	6.525071
H	-4.892894	5.318912	6.670190
H	-6.015813	3.747147	5.060748
H	-4.639435	2.589122	3.305830
H	-0.161235	-2.215069	2.915854
H	-0.670114	-0.969816	-3.702253
H	-4.687466	2.184747	-1.924138
H	-0.307979	3.959856	4.025354
H	-4.318691	-4.279557	3.153604
H	-3.090179	-5.451604	3.756816
H	-3.610907	-4.104811	4.799353
H	-2.908546	-3.845086	1.094559
H	-1.219803	-3.281712	1.235547
H	-1.632515	-4.974953	1.655482
H	-3.673414	-1.897746	2.658178
H	-2.861265	-1.667051	4.240523
H	-1.983705	-1.340502	2.715001
H	-1.337115	-4.988835	-3.819076
H	-0.443696	-4.582779	-5.295865
H	4.982861	-5.653101	-2.840239
H	1.330073	-5.594437	-6.334253
H	0.585773	-4.141846	-0.248789
H	-0.068647	-2.922281	-1.384188
H	-0.824625	-4.540363	-1.300798
H	5.874593	-7.487318	-5.710027
H	6.279675	-5.806535	-6.119757
H	6.547126	-6.404297	-4.452874
H	4.513243	-5.801144	-7.789863
H	4.099736	-7.477120	-7.375348
H	2.824553	-6.370407	-7.971482
H	-4.768059	-0.224230	0.456055
H	-3.913094	1.322091	0.175880
H	-5.486328	0.966121	-0.643631
H	-4.996543	-1.941092	-1.455819
H	-5.528745	-0.698344	-2.636699
H	-4.063400	-1.697083	-2.975003
H	-2.811926	-1.620981	-0.152944
H	-1.918968	-1.329016	-1.683904
H	-1.846413	-0.121104	-0.360527
H	1.848625	6.158061	4.617700
H	2.132246	5.169419	6.062494

H	3.458909	1.703553	0.874832
H	1.002429	5.925247	2.185958
H	1.658328	2.502767	6.588308
H	3.086691	1.493699	6.169620
H	3.305272	3.200503	6.691281
H	3.644128	4.048168	-1.602766
H	3.301374	2.298999	-1.418718
H	2.016510	3.419744	-1.949202
H	0.586956	5.148750	-1.198907
H	0.765040	6.532152	-0.075671
H	2.121076	6.054070	-1.148257

Conformation 33.
Multiplicity: 2
Charge: 0
E(B97-3c) = -5613.030013708073 Hartree
E(M06/def2-TZVP) = -5612.885498672970 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -5610.945197813673 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -5611.179011379139 Hartree
E(PBEh-3c) = -5604.827598142869 Hartree
E(PM6) = 171.04173 Kcal/mol
E(PM7) = 51.00600 Kcal/mol
E(ωB97X-V/def2-TZVP) = -5614.584317043254 Hartree
E(GFN1-xTB) = -265.551105162363 Hartree
E(GFN2-xTB) = -259.272104016133 Hartree
E(GFN-FF) = -33.823526285600 Hartree

Coordinates:

Cu	-0.465208	0.669407	0.054689
N	-2.298700	-0.147250	-0.166549
N	-0.730723	0.698676	2.062061
N	1.234752	1.733250	0.260948
N	-0.305913	0.837166	-1.963209
C	-2.817030	-0.669557	-1.329869
C	-3.231748	-0.378756	0.820388
C	-1.857398	0.338020	2.765583
C	0.246611	0.967542	2.992176
C	1.960434	1.863643	1.424354
C	1.964333	2.341222	-0.732710
C	0.598030	1.598818	-2.671350
C	-1.076675	0.176280	-2.892588
C	-4.120239	-1.256334	-1.072440
C	-4.392008	-1.046089	0.257730
C	-1.592709	0.402012	4.192318
C	-0.272396	0.753327	4.332278
C	3.203869	2.561831	1.154780
C	3.191393	2.887620	-0.181166
C	0.380183	1.425316	-4.097579
C	-0.622794	0.498816	-4.234298
C	-3.068051	-0.113734	2.197303
C	1.539025	1.456065	2.707099
C	1.631878	2.375566	-2.108429
C	-2.218951	-0.601677	-2.608456
O	-6.911795	3.115907	2.656179
O	4.679660	-2.253173	4.003224
O	1.594200	7.370835	-1.548809
O	-1.646132	-5.598714	-3.135228
N	-5.050459	1.810352	2.300747
N	3.400304	-0.583852	3.038230
N	2.777665	-3.766656	2.009579
N	1.039132	-5.053766	2.673943
N	1.278567	5.101884	-1.780635
N	-1.671009	-3.305790	-2.794241
N	0.341286	-3.481313	-0.946103
N	0.805137	-1.553683	0.135275
C	-4.247431	-0.314175	3.095098
C	-5.251681	0.696906	3.127525
C	-6.374733	0.543744	3.968283
C	-6.490270	-0.603654	4.764707
C	-5.506231	-1.604761	4.741342
C	-4.389308	-1.452687	3.905522
C	2.523481	1.523094	3.830018
C	3.436363	0.443380	3.998180
C	4.327301	0.440036	5.092652
C	4.322320	1.514681	5.992163
C	3.442767	2.594889	5.822279
C	2.545522	2.589731	4.743505
C	2.402996	3.324126	-2.966103
C	2.213164	4.724439	-2.754711
C	2.948170	5.656069	-3.517577
C	3.852464	5.199828	-4.486091
C	4.036615	3.826824	-4.713186
C	3.310805	2.898847	-3.951467
C	-2.842880	-1.408843	-3.704063
C	-2.559597	-2.804398	-3.757777
C	-3.156615	-3.611493	-4.747807
C	-4.019727	-3.027043	-5.684636
C	-4.297611	-1.651559	-5.650737
C	-3.708962	-0.851358	-4.659242
C	-5.839946	2.921383	2.088523
C	-5.221823	3.955466	1.104327
C	-6.381267	4.682524	0.403932
C	-4.297247	3.314208	0.049768
C	-4.420870	4.956129	1.968626
C	3.983376	-1.831078	3.085798
C	3.702619	-2.659739	1.824259
C	2.722103	-4.836566	1.122605
C	1.636002	-5.638695	1.568416
C	1.310136	-6.809903	0.860368
C	2.035731	-7.146635	-0.294935
C	3.104263	-6.304159	-0.749108
C	3.453410	-5.145926	-0.030885
C	1.723837	-3.942224	2.911196
C	1.372793	-2.979301	3.996034
C	1.666609	-8.379448	-1.083539
C	3.849013	-6.647203	-2.014986
C	1.053717	6.328107	-1.189082
C	0.106644	6.274603	0.043863
C	1.031504	6.256765	1.282939
C	-0.743021	7.556393	0.037219
C	-0.812898	5.038903	0.071583
C	-1.278298	-4.595512	-2.533913
C	-0.310953	-4.712005	-1.337164
C	1.422620	-2.913711	-1.615756
C	1.703030	-1.710939	-0.919302
C	2.795500	-0.922793	-1.324216
C	3.581934	-1.340182	-2.410237
C	3.273408	-2.553869	-3.109134
C	2.180808	-3.342581	-2.710949
C	0.015453	-2.627208	0.104905
C	-1.073527	-2.937464	1.070149
C	4.764751	-0.507248	-2.837254
C	4.129934	-2.995689	-4.268445
H	-4.748598	-1.739371	-1.828745
H	-5.283262	-1.333772	0.826139
H	-2.325866	0.180757	4.975135
H	0.300239	0.889378	5.255879
H	3.968455	2.791586	1.905232
H	3.948462	3.430060	-0.757962
H	0.942965	1.937032	-4.885023
H	-1.055761	0.095228	-5.155762
H	-7.132745	1.336057	3.974464
H	-7.369860	-0.713402	5.417253
H	-5.607570	-2.502751	5.368337
H	-3.607323	-2.226559	3.868686
H	5.000119	-0.415682	5.222013
H	5.022977	1.503035	6.840736
H	3.449041	3.436413	6.530543
H	1.837425	3.419682	4.598880
H	2.792023	6.724541	-3.325750
H	4.420971	5.935812	-5.074849
H	4.749055	3.477319	-5.474950
H	3.456452	1.818994	-4.099684
H	-2.929992	-4.684645	-4.758602
H	-4.482151	-3.662696	-6.454950
H	-4.976912	-1.201667	-6.389668
H	-3.925690	0.226375	-4.608195
H	-4.188493	1.767225	1.752322
H	2.766718	-0.410695	2.249307
H	0.774702	4.317562	-1.361772
H	-1.254142	-2.585835	-2.195135
H	-5.994956	5.524081	-0.205374
H	-6.936568	3.994999	-0.265513
H	-7.096727	5.073056	1.151199
H	-3.967862	4.086045	-0.674774
H	-3.365683	2.886189	0.479647
H	-4.811458	2.514764	-0.521671
H	-3.997477	5.761023	1.332620
H	-5.074663	5.423512	2.731147
H	-3.581563	4.455446	2.494369
H	3.352148	-2.015637	0.990582
H	4.680772	-3.088229	1.526699
H	0.479286	-7.443995	1.205491
H	4.257857	-4.493063	-0.401567
H	0.511728	-3.397532	4.546212
H	2.210786	-2.826382	4.704724
H	1.086448	-1.985965	3.593764
H	1.303551	-8.124464	-2.103340
H	2.533204	-9.059643	-1.221504
H	0.863967	-8.951540	-0.580588
H	4.366875	-7.627180	-1.938331
H	3.165259	-6.728697	-2.887438
H	4.609389	-5.879438	-2.255067
H	0.425216	6.273463	2.212208
H	1.663852	5.344590	1.300356
H	1.698297	7.141328	1.283131
H	-1.324806	7.638772	0.977570
H	-0.093292	8.445721	-0.065568
H	-1.456476	7.557040	-0.812002
H	-1.510410	5.111428	0.929799
H	-1.429714	4.958611	-0.847042
H	-0.260114	4.084660	0.210846

H	-0.868558	-5.123512	-0.473610
H	0.451437	-5.473381	-1.592132
H	3.039944	0.009106	-0.795799
H	1.948757	-4.277360	-3.242286
H	-0.842580	-3.865585	1.636313
H	-1.155496	-2.104335	1.787676
H	-2.053802	-3.062218	0.565752
H	4.707709	-0.226891	-3.910448
H	4.830838	0.426347	-2.246780
H	5.722794	-1.057026	-2.715447
H	5.192214	-3.123592	-3.969702
H	3.779064	-3.959066	-4.685088
H	4.126785	-2.249670	-5.091621

Conformation 34.
Multiplicity: 2
Charge: 0
E(B97-3c) = -5612.992167069223 Hartree
E(M06/def2-TZVP) = -5612.852003395962 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -5610.904860312198 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -5611.138181448125 Hartree
E(PBEh-3c) = -5604.793236070004 Hartree
E(PM6) = 205.14573 Kcal/mol
E(PM7) = 88.65215 Kcal/mol
E(ωB97X-V/def2-TZVP) = -5614.549365030531 Hartree
E(GFN1-xTB) = -265.512834951264 Hartree
E(GFN2-xTB) = -259.246268615672 Hartree
E(GFN-FF) = -33.782771217145 Hartree

Coordinates:

Cu	-0.958062	-0.782300	-0.525896
N	0.645183	-1.993010	-0.755282
N	-0.435994	-0.463933	1.410389
N	-2.558504	0.440629	-0.293050
N	-1.483387	-1.076192	-2.462910
C	1.063471	-2.586454	-1.929849
C	1.531141	-2.401950	0.218130
C	0.611734	-1.054597	2.086142
C	-0.991389	0.458143	2.275378
C	-2.835535	1.230152	0.803170
C	-3.550637	0.692556	-1.216868
C	-2.646880	-0.664852	-3.085480
C	-0.788941	-1.812495	-3.398097
C	2.251644	-3.385838	-1.690425
C	2.524361	-3.291501	-0.352530
C	0.715225	-0.498663	3.419546
C	-0.271913	0.448767	3.534045
C	-4.042670	1.995745	0.571403
C	-4.492844	1.653858	-0.682700
C	-2.692357	-1.170422	-4.443033
C	-1.522011	-1.852370	-4.649755
C	1.515668	-2.000553	1.564844
C	-2.083212	1.298404	1.991248
C	-3.639301	0.146377	-2.513655
C	0.429650	-2.486663	-3.182201
O	0.382206	-4.621910	1.766389
O	0.182956	3.667974	-0.256899
O	-5.154050	-2.798181	-2.949874
O	3.814005	-0.047892	-6.018348
N	0.883362	-3.771757	3.830793
N	-1.481882	3.975092	1.269186
N	0.818510	4.896935	2.919841
N	0.660710	6.184954	4.774835
N	-6.073718	-1.081084	-1.760227
N	2.442724	-1.082189	-4.466375
N	3.982228	0.410710	-2.591704
N	4.079721	-0.264078	-0.439818
C	2.555480	-2.533096	2.492917
C	2.219332	-3.369199	3.590316
C	3.222398	-3.763308	4.498055
C	4.546205	-3.336498	4.332225
C	4.884086	-2.515810	3.244556
C	3.893556	-2.118183	2.335949
C	-2.395398	2.408627	2.940394
C	-2.064729	3.737561	2.555892
C	-2.321109	4.813237	3.422316
C	-2.894465	4.583255	4.680741
C	-3.228716	3.275847	5.068692
C	-2.983103	2.198483	4.203286
C	-4.884521	0.424696	-3.289083
C	-6.096261	-0.184554	-2.872693
C	-7.291702	0.077186	-3.557941
C	-7.298340	0.947102	-4.658785
C	-6.102849	1.547047	-5.082917
C	-4.903958	1.285651	-4.401986
C	1.103677	-3.080196	-4.380905
C	2.090813	-2.307342	-5.055150
C	2.674891	-2.785523	-6.246122
C	2.297598	-4.040824	-6.741670
C	1.346239	-4.825357	-6.070907
C	0.751073	-4.337652	-4.897159
C	0.023493	-4.333080	2.902556
C	-1.446187	-4.484187	3.373902
C	-2.102319	-5.579711	2.519686
C	-2.129725	-3.122431	3.106977
C	-1.566584	-4.843930	4.866406
C	-0.165965	3.773626	0.917024
C	0.860351	3.728583	2.065175
C	0.832121	6.215740	2.475010
C	0.726198	7.003080	3.655255
C	0.707686	8.405219	3.544794
C	0.792403	9.001344	2.276402
C	0.897877	8.189287	1.098952
C	0.919444	6.786576	1.197089
C	0.718684	4.948146	4.312811
C	0.657753	3.722679	5.159781
C	0.775514	10.504753	2.147825
C	0.989258	8.842078	-0.257695
C	-5.440792	-2.307545	-1.862157
C	-5.117805	-3.040198	-0.535417
C	-5.402772	-2.208770	0.725764
C	-5.959805	-4.332549	-0.526581
C	-3.619019	-3.399810	-0.592741
C	3.280123	-0.091701	-4.914678
C	3.525868	0.992580	-3.837517
C	5.141489	-0.352233	-2.478054
C	5.183300	-0.761091	-1.119506
C	6.245275	-1.572697	-0.681019
C	7.239236	-1.962444	-1.592959
C	7.176380	-1.539322	-2.961736
C	6.118950	-0.727582	-3.409504
C	3.374956	0.416796	-1.331300
C	2.080615	1.104501	-1.055810
C	8.378726	-2.838546	-1.134205
C	8.245243	-1.974009	-3.932636
H	2.781327	-3.961227	-2.457247
H	3.325276	-3.774802	0.213930
H	1.472221	-0.782431	4.157965
H	-0.500642	1.081153	4.396780
H	-4.494992	2.689761	1.289212
H	-5.371493	2.032905	-1.216364
H	-3.530108	-1.028905	-5.132432
H	-1.188126	-2.374049	-5.552409
H	2.950022	-4.423408	5.336075
H	5.314794	-3.651689	5.054097
H	5.919939	-2.167563	3.112166
H	4.114995	-1.432007	1.500328
H	-2.042224	5.828143	3.103299
H	-3.070225	5.429433	5.360711
H	-3.684779	3.092447	6.053250
H	-3.249466	1.172785	4.499601
H	-8.211714	-0.422820	-3.222158
H	-8.239128	1.149555	-5.192345
H	-6.102545	2.226711	-5.948348
H	-3.965235	1.761695	-4.722844
H	3.409619	-2.156093	-6.762459
H	2.759848	-4.409856	-7.669852
H	1.059429	-5.811571	-6.464689
H	-0.011540	-4.928790	-4.368301
H	0.562855	-3.732412	4.798861
H	-2.111427	3.911047	0.460081
H	-6.162797	-0.669627	-0.828787
H	2.071600	-0.962417	-3.517978
H	-3.192058	-5.623774	2.719275
H	-1.936649	-5.375972	1.445687
H	-1.667221	-6.575426	2.739252
H	-3.209719	-3.184103	3.355449
H	-1.678655	-2.314014	3.717269
H	-2.034452	-2.829385	2.044076
H	-2.630819	-5.018526	5.124952
H	-1.005566	-5.767593	5.116378
H	-1.221131	-4.026053	5.535007
H	0.678787	2.824943	2.680195
H	1.851141	3.618871	1.579074
H	0.630764	9.022780	4.452491
H	1.002062	6.166785	0.291876
H	0.712570	4.036139	6.216943
H	-0.298274	3.179052	5.009594
H	1.488216	3.018445	4.948704
H	1.689912	10.886369	1.645370
H	-0.083171	10.859047	1.537741
H	0.707275	10.992085	3.139200
H	0.111138	9.490872	-0.463389
H	1.882898	9.497479	-0.340392
H	1.048526	8.087698	-1.065382
H	-5.118267	-2.786727	1.628399
H	-4.809141	-1.270528	0.746581
H	-6.480057	-1.959942	0.830200
H	-5.697749	-4.958615	0.351040
H	-7.044878	-4.105714	-0.478848
H	-5.768930	-4.915278	-1.448310
H	-3.353246	-4.074144	0.244743

H	-3.381464	-3.902702	-1.548907
H	-2.982907	-2.493528	-0.520460
H	4.284410	1.684814	-4.254165
H	2.598290	1.569030	-3.648401
H	6.293272	-1.907278	0.366085
H	6.061267	-0.418486	-4.463944
H	1.259865	0.736030	-1.707711
H	1.790113	0.886016	-0.013213
H	2.123589	2.206405	-1.175003
H	9.364298	-2.349955	-1.290095
H	8.290105	-3.083641	-0.058470
H	8.415295	-3.795911	-1.696776
H	8.302964	-3.080736	-4.012445
H	8.056511	-1.572829	-4.946624
H	9.254228	-1.633681	-3.615462

Conformation 6.
Multiplicity: 2
Charge: 0
E(B97-3c) = -5613.008101273340 Hartree
E(M06/def2-TZVP) = -5612.865506457643 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -5610.925946595728 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -5611.158100151668 Hartree
E(PBEh-3c) = -5604.810234962992 Hartree
E(PM6) = 174.12711 Kcal/mol
E(PM7) = 73.59270 Kcal/mol
E(ωB97X-V/def2-TZVP) = -5614.563505922404 Hartree
E(GFN1-xTB) = -265.522367452833 Hartree
E(GFN2-xTB) = -259.255506262497 Hartree
E(GFN-FF) = -33.808088401167 Hartree

Coordinates:

Cu	-1.951721	-1.104665	0.916956
N	-2.995400	0.556304	1.380629
N	-3.153684	-1.396874	-0.676268
N	-0.896758	-2.755224	0.438086
N	-0.751932	-0.798893	2.509193
C	-2.621682	1.538658	2.274921
C	-4.174106	0.976125	0.804057
C	-4.376896	-0.802299	-0.912103
C	-2.976006	-2.335528	-1.668971
C	-0.968399	-3.465851	-0.741982
C	0.069229	-3.370489	1.208475
C	0.211326	-1.656248	2.999302
C	-0.708065	0.331198	3.300231
C	-3.566164	2.637154	2.224480
C	-4.544321	2.274870	1.330730
C	-5.003288	-1.408082	-2.069541
C	-4.115192	-2.330131	-2.565515
C	-0.008529	-4.554251	-0.723111
C	0.596997	-4.525831	0.507313
C	0.876613	-1.054341	4.139890
C	0.315765	0.186001	4.317230
C	-4.894505	0.296525	-0.200406
C	-1.895691	-3.239033	-1.779263
C	0.581022	-2.894604	2.434735
C	-1.539139	1.463458	3.174381
O	-6.247736	-1.787492	1.101798
O	-1.377172	-1.201355	-6.351272
O	5.311486	-3.598544	0.736934
O	2.087874	4.941061	2.370487
N	-7.095868	0.245437	1.722475
N	-1.207331	-1.900420	-4.152462
N	-0.341835	0.804288	-3.594392
N	0.544296	1.845353	-1.793546
N	3.206566	-2.943551	1.401117
N	0.577319	3.195803	2.555040
N	3.164023	3.856030	0.025515
N	3.893496	5.332893	-1.526164
C	-6.249810	0.816159	-0.532869
C	-7.287533	0.808321	0.440595
C	-8.526827	1.409246	0.142378
C	-8.755101	2.008281	-1.102223
C	-7.747060	1.996434	-2.078551
C	-6.510890	1.404700	-1.787296
C	-1.762797	-3.995374	-3.059236
C	-1.421754	-3.289168	-4.249927
C	-1.319285	-3.982234	-5.474260
C	-1.548551	-5.363650	-5.513696
C	-1.881255	-6.071130	-4.348551
C	-1.986430	-5.382775	-3.131896
C	1.662650	-3.681949	3.105229
C	2.978078	-3.703409	2.555599
C	3.986141	-4.466268	3.184748
C	3.691069	-5.181023	4.352919
C	2.404857	-5.150002	4.913852
C	1.400246	-4.400262	4.285083
C	-1.252256	2.651180	4.036760
C	-0.178072	3.521124	3.691894
C	0.084103	4.659513	4.484844
C	-0.710204	4.920482	5.608861
C	-1.768643	4.068257	5.960409
C	-2.033055	2.940762	5.169309
C	-6.564624	-1.008450	1.992948
C	-6.345424	-1.313682	3.496064
C	-6.133683	-2.827559	3.644772
C	-7.545339	-0.867144	4.354649
C	-5.069668	-0.560583	3.940373
C	-1.274724	-0.960745	-5.153300
C	-1.290972	0.495743	-4.644311
C	1.043393	0.772646	-3.768133
C	1.577674	1.437674	-2.634904
C	2.966883	1.624863	-2.539690
C	3.803967	1.130188	-3.552438
C	3.247747	0.428281	-4.672510
C	1.855260	0.257013	-4.787360
C	-0.578799	1.478848	-2.391417
C	-1.951894	1.752201	-1.880818
C	5.293400	1.353248	-3.458508
C	4.158438	-0.116858	-5.742534
C	4.296646	-2.932384	0.549618
C	4.158675	-1.934461	-0.629986
C	4.679632	-0.579772	-0.100943
C	5.051577	-2.428108	-1.778863
C	2.708324	-1.783597	-1.134035
C	1.645222	3.865382	1.990064
C	2.235723	3.081530	0.804923
C	4.538087	3.670835	-0.061476
C	4.970233	4.599756	-1.050904
C	6.327452	4.624177	-1.420397
C	7.228848	3.728971	-0.821412
C	6.774518	2.801519	0.173277
C	5.422072	2.778852	0.558421
C	2.838696	4.871036	-0.877376
C	1.433414	5.332285	-1.058445
C	8.682790	3.737522	-1.225744
C	7.746113	1.836579	0.805336
H	-3.486468	3.557417	2.812602
H	-5.425776	2.847276	1.022416
H	-6.002912	-1.164212	-2.442029
H	-4.233511	-2.993028	-3.429542
H	0.156667	-5.262363	-1.541209
H	1.359448	-5.204962	0.903387
H	1.679296	-1.529013	4.714082
H	0.553241	0.940835	5.074868
H	-9.323148	1.386718	0.902248
H	-9.728977	2.474700	-1.313152
H	-7.917611	2.460388	-3.061139
H	-5.700882	1.422955	-2.531867
H	-1.073289	-3.417665	-6.380733
H	-1.465876	-5.891861	-6.475596
H	-2.067748	-7.154452	-4.386373
H	-2.269163	-5.916684	-2.212393
H	4.984704	-4.481862	2.732354
H	4.487218	-5.770206	4.833129
H	2.180872	-5.711729	5.832620
H	0.382104	-4.369958	4.701829
H	0.907511	5.322337	4.193570
H	-0.493853	5.810444	6.219235
H	-2.386195	4.278700	6.845969
H	-2.857567	2.257553	5.424617
H	-7.507372	0.752212	2.507261
H	-1.140850	-1.535628	-3.196869
H	2.404518	-2.389383	1.092953
H	0.288421	2.329729	2.089377
H	-5.898443	-3.077578	4.698656
H	-7.038314	-3.392244	3.343680
H	-5.302147	-3.168609	3.000199
H	-7.391799	-1.181671	5.406803
H	-7.670909	0.236930	4.380446
H	-8.494378	-1.319818	4.002317
H	-4.860197	-0.768662	5.009966
H	-4.190671	-0.879334	3.346890
H	-5.174242	0.536111	3.813717
H	-1.109863	1.128716	-5.537085
H	-2.313224	0.712721	-4.273620
H	3.400233	2.168507	-1.691778
H	1.430197	-0.259551	-5.661360
H	-1.874169	2.237133	-0.891851
H	-2.516846	2.430695	-2.554697
H	-2.541681	0.822686	-1.755878
H	5.853423	0.394185	-3.425545
H	5.677992	1.909332	-4.339330
H	5.559594	1.935789	-2.555831
H	4.758382	0.687523	-6.218608
H	4.889586	-0.841966	-5.325625
H	3.587257	-0.631272	-6.538581
H	4.658970	0.184616	-0.900422
H	4.051700	-0.211160	0.736419
H	5.720844	-0.670752	0.266929
H	5.062213	-1.679379	-2.595638
H	6.085001	-2.599216	-1.424407

H	4.675302	-3.385474	-2.192407
H	2.693988	-1.151516	-2.043410
H	2.256896	-2.763685	-1.388889
H	2.040150	-1.272928	-0.406369
H	2.766561	2.192669	1.206266
H	1.426758	2.687244	0.143210
H	6.668325	5.336984	-2.186420
H	5.085142	2.067780	1.327894
H	1.040479	5.789205	-0.126195
H	1.415362	6.088515	-1.862730
H	0.770197	4.486052	-1.337287
H	9.004488	2.755819	-1.635371
H	8.879524	4.505077	-1.998441
H	9.351311	3.947439	-0.363461
H	8.586215	2.361327	1.308276
H	7.248008	1.198107	1.560049
H	8.208119	1.164913	0.050009

Conformation 8.
Multiplicity: 2
Charge: 0
E(B97-3c) = -5613.025490200966 Hartree
E(M06/def2-TZVP) = -5612.885267637605 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -5610.941511635044 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -5611.174233123637 Hartree
E(PBEh-3c) = -5604.827478043128 Hartree
E(PM6) = 189.76412 Kcal/mol
E(PM7) = 60.34417 Kcal/mol
E(ωB97X-V/def2-TZVP) = -5614.580917187273 Hartree
E(GFN1-xTB) = -265.543211639934 Hartree
E(GFN2-xTB) = -259.274736636298 Hartree
E(GFN-FF) = -33.831225456046 Hartree

Coordinates:

Cu	0.399218	-0.512176	1.051048
N	-1.182084	-1.714729	1.482698
N	1.141866	-1.938041	-0.170454
N	2.006020	0.671874	0.658846
N	-0.378528	0.941199	2.222755
C	-2.203331	-1.445495	2.373586
C	-1.476432	-2.938530	0.916111
C	0.536537	-3.127417	-0.525895
C	2.365348	-1.919796	-0.811723
C	3.135609	0.318231	-0.054272
C	2.238247	1.947402	1.135593
C	0.116021	2.221547	2.393058
C	-1.538697	0.873502	2.969902
C	-3.154984	-2.540242	2.386217
C	-2.717777	-3.453309	1.460999
C	1.395106	-3.870803	-1.428845
C	2.530640	-3.123452	-1.602729
C	4.106909	1.395393	-0.019879
C	3.548929	2.406282	0.719731
C	-0.780104	2.992171	3.232066
C	-1.801435	2.152803	3.599215
C	-0.705104	-3.604010	-0.055404
C	3.327828	-0.893841	-0.744582
C	1.354105	2.707603	1.924107
C	-2.374755	-0.252429	3.103139
O	-0.375152	-4.651960	-4.596548
O	4.253661	0.714603	-5.477715
O	2.754436	3.897746	6.638976
O	-7.036348	1.160275	1.678188
N	-1.483916	-3.793745	-2.783065
N	3.699815	0.264544	-3.274611
N	2.366756	2.783956	-3.422672
N	1.825437	3.954362	-1.567926
N	2.248965	3.084602	4.545838
N	-4.930046	0.277873	2.071233
N	-4.895187	-0.460047	-0.653032
N	-3.297607	-1.848264	-1.430414
C	-1.201113	-4.890854	-0.625987
C	-1.506256	-4.973569	-2.012182
C	-1.849572	-6.218061	-2.580035
C	-1.932108	-7.361120	-1.774658
C	-1.676990	-7.279323	-0.395823
C	-1.307862	-6.050543	0.167713
C	4.599972	-1.103161	-1.507811
C	4.745421	-0.549649	-2.809806
C	5.901499	-0.821462	-3.570744
C	6.914979	-1.619886	-3.024703
C	6.793230	-2.156339	-1.733487
C	5.634050	-1.899367	-0.986728
C	1.787177	4.063326	2.388288
C	2.223615	4.228859	3.735768
C	2.612912	5.506702	4.191818
C	2.572030	6.597641	3.312785
C	2.153207	6.439137	1.982152
C	1.763521	5.170985	1.523911
C	-3.560042	-0.122119	4.010294
C	-4.839839	0.184590	3.470048
C	-5.941835	0.391669	4.324840
C	-5.769828	0.277250	5.710901
C	-4.516096	-0.037798	6.257554
C	-3.419180	-0.230621	5.404435
C	-0.884941	-3.691224	-4.023837
C	-0.902900	-2.266545	-4.635661
C	-0.088213	-2.292271	-5.935404
C	-0.275059	-1.255973	-3.654368
C	-2.366298	-1.873118	-4.931981
C	3.536947	0.872174	-4.495350
C	2.325825	1.831816	-4.513534
C	3.384484	3.718323	-3.242405
C	3.022829	4.440613	-2.074454
C	3.873118	5.457020	-1.603130
C	5.060252	5.738557	-2.297982
C	5.404668	5.000949	-3.479292
C	4.560978	3.982014	-3.956649
C	1.464759	2.968277	-2.371015
C	0.270832	2.100530	-2.161723
C	5.984897	6.819685	-1.795655
C	6.685166	5.311415	-4.212448
C	2.468825	2.956970	5.903330
C	2.338416	1.493405	6.413202
C	3.479095	0.650122	5.800861
C	2.467421	1.513445	7.942158
C	0.971335	0.897469	6.010243
C	-5.953936	0.740822	1.284890
C	-5.592595	0.732350	-0.218419
C	-5.500382	-1.706567	-0.793166
C	-4.485754	-2.561784	-1.292841
C	-4.784362	-3.914673	-1.533974
C	-6.076547	-4.390861	-1.262339
C	-7.088440	-3.510305	-0.753041
C	-6.798198	-2.155048	-0.517418
C	-3.562894	-0.610092	-1.032381
C	-2.574427	0.503630	-0.959244
C	-6.397863	-5.845148	-1.502655
C	-8.468887	-4.040882	-0.462060
H	-4.055682	-2.582942	3.008349
H	-3.196003	-4.388557	1.154839
H	1.154306	-4.841794	-1.873714
H	3.409742	-3.356587	-2.212240
H	5.087027	1.370261	-0.508686
H	3.967219	3.389307	0.957317
H	-0.626678	4.041766	3.504424
H	-2.665958	2.370402	4.235150
H	-2.047871	-6.270040	-3.657788
H	-2.204337	-8.325539	-2.229758
H	-1.744588	-8.176370	0.237370
H	-1.063370	-5.981257	1.238356
H	5.975943	-0.406046	-4.582674
H	7.814554	-1.825402	-3.624465
H	7.593572	-2.781356	-1.310907
H	5.510581	-2.327386	0.019350
H	2.936784	5.613069	5.233850
H	2.876687	7.589477	3.680868
H	2.123989	7.302148	1.299605
H	1.448839	5.004858	0.480780
H	-6.910984	0.651709	3.882608
H	-6.634360	0.439460	6.372271
H	-4.388943	-0.126513	7.346485
H	-2.424446	-0.460627	5.815499
H	-1.881684	-2.949577	-2.322870
H	3.012957	0.508130	-2.553377
H	1.982093	2.227143	4.056699
H	-4.099935	-0.067115	1.578206
H	-0.102700	-1.291397	-6.413438
H	0.964195	-2.575923	-5.739643
H	-0.498827	-3.032728	-6.647647
H	-0.299180	-0.242602	-4.107152
H	-0.826420	-1.202795	-2.696150
H	0.779058	-1.512491	-3.424671
H	-2.398317	-0.879553	-5.426474
H	-2.842125	-2.605554	-5.614872
H	-2.974032	-1.815008	-4.007273
H	2.349057	2.348704	-5.493448
H	1.386158	1.247729	-4.449889
H	3.614018	6.015890	-0.691621
H	4.835593	3.405847	-4.853219
H	-0.303422	2.513605	-1.313812
H	-0.388461	2.050073	-3.052468
H	0.559667	1.061049	-1.895966
H	6.996375	6.422556	-1.564603
H	6.131917	7.621447	-2.550518
H	5.589380	7.290365	-0.875468
H	6.714765	6.366055	-4.560294
H	7.574944	5.175408	-3.561304
H	6.811265	4.658998	-5.097273
H	3.435962	-0.387778	6.190769
H	3.413831	0.593092	4.694630
H	4.470520	1.072439	6.060712

H	2.414646	0.481352	8.343413
H	3.426564	1.969767	8.251776
H	1.657908	2.113379	8.401497
H	0.859072	-0.115275	6.449764
H	0.132742	1.523861	6.375232
H	0.850774	0.783226	4.912569
H	-6.544585	0.842970	-0.773322
H	-4.968882	1.620861	-0.442683
H	-4.015352	-4.597949	-1.918480
H	-7.568191	-1.481067	-0.112015
H	-2.598294	1.026954	0.018697
H	-1.562947	0.080087	-1.080295
H	-2.733990	1.262576	-1.753856
H	-7.207335	-5.970280	-2.253177
H	-5.508864	-6.396057	-1.864704
H	-6.752757	-6.345972	-0.576943
H	-8.443195	-4.861203	0.286437
H	-9.134582	-3.247867	-0.071500
H	-8.944413	-4.466476	-1.371204

LIBLEN

Conformation 1.
Multiplicity: 3
Charge: 0
E(B97-3c) = -2729.966866050881 Hartree
E(M06/def2-TZVP) = -2729.937241457135 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -2728.978699280144 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -2729.126280344690 Hartree
E(PBEh-3c) = -2726.115674076072 Hartree
E(PM6) = 93.42146 Kcal/mol
E(PM7) = 107.36848 Kcal/mol
E(ωB97X-V/def2-TZVP) = -2730.727815661306 Hartree
E(GFN1-xTB) = -120.621411026550 Hartree
E(GFN2-xTB) = -119.812202924278 Hartree
E(GFN-FF) = -16.973041167079 Hartree

Coordinates:

V	0.148242	-0.026838	0.006472
O	-1.054991	1.361986	-1.016424
N	-1.096676	-0.835887	1.270135
N	0.478053	-1.000775	-1.686449
N	1.462319	1.201804	0.773012
C	2.017137	0.401549	1.784226
C	2.183254	-0.983524	1.516250
C	2.476117	-1.888298	2.550522
C	2.684776	-1.422505	3.853281
C	2.584644	-0.040640	4.117271
C	2.244795	0.864002	3.108646
C	1.738074	2.576796	0.712828
C	0.704722	3.526644	0.523306
C	0.999984	4.893088	0.412822
C	2.324448	5.348976	0.503334
C	3.355829	4.415967	0.710110
C	3.071705	3.049311	0.812104
C	1.764273	-1.456480	-2.043302
C	1.963244	-2.750839	-2.589385
C	3.252044	-3.212787	-2.879319
C	4.376285	-2.406289	-2.627466
C	4.191175	-1.124028	-2.088176
C	2.902675	-0.646767	-1.809182
C	-0.588162	-1.232793	-2.572059
C	-1.889980	-1.486411	-2.069431
C	-2.987391	-1.598902	-2.933881
C	-2.818577	-1.488147	-4.324117
C	-1.527573	-1.269310	-4.837945
C	-0.427442	-1.142006	-3.981436
C	-2.084969	-0.005905	1.835610
C	-3.446007	-0.399826	1.877220
C	-4.428118	0.488637	2.330332
C	-4.080111	1.784581	2.756674
C	-2.731544	2.173352	2.747028
C	-1.739594	1.283773	2.305100
C	-0.915662	-2.141379	1.759139
C	-0.342883	-3.136911	0.926773
C	-0.074376	-4.418009	1.423388
C	-0.383931	-4.750481	2.752788
C	-0.966682	-3.775376	3.580462
C	-1.229065	-2.487810	3.097761
C	-0.467672	2.029558	-2.176591
C	-1.553037	2.984773	-2.652870
C	-2.830777	2.198082	-2.328049
C	-2.498583	1.583113	-0.974936
H	2.135135	-1.351848	0.475670
H	2.551897	-2.961056	2.320101
H	2.929929	-2.125693	4.662523
H	2.752382	0.332964	5.139643
H	2.126688	1.934637	3.331250
H	-0.334726	3.174011	0.482183
H	0.178196	5.612248	0.269176
H	2.552173	6.421994	0.420277
H	4.399899	4.757821	0.784821
H	3.881421	2.319979	0.965103
H	1.086846	-3.389701	-2.774796
H	3.382394	-4.223346	-3.296928
H	5.387844	-2.776170	-2.851503
H	5.059594	-0.477088	-1.889830
H	2.757971	0.362852	-1.393927
H	-2.021238	-1.598120	-0.981853
H	-3.986061	-1.794918	-2.512930
H	-3.679500	-1.586798	-5.001811
H	-1.375852	-1.186950	-5.925647
H	0.576923	-0.959618	-4.391974
H	-3.716380	-1.409069	1.531490
H	-5.482451	0.171097	2.343517
H	-4.857429	2.479532	3.108032
H	-2.440533	3.174605	3.100813
H	-0.677366	1.568954	2.323935
H	-0.103251	-2.885060	-0.117118
H	0.374545	-5.168998	0.754815
H	-0.177658	-5.759591	3.139398
H	-1.211177	-4.017005	4.626708
H	-1.660649	-1.724196	3.760844
H	0.461986	2.527794	-1.839765
H	-0.229372	1.258005	-2.936932
H	-1.515262	3.933266	-2.076928
H	-1.447641	3.228034	-3.727549
H	-3.738642	2.830254	-2.284757
H	-2.995528	1.398224	-3.079608
H	-2.988750	0.611033	-0.788833
H	-2.716347	2.260852	-0.123186

Conformation 16.
Multiplicity: 3
Charge: 0
E(B97-3c) = -2729.964561799386 Hartree
E(M06/def2-TZVP) = -2729.930628848846 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -2728.975017083584 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -2729.122424078092 Hartree
E(PBEh-3c) = -2726.114025205031 Hartree
E(PM6) = 96.23616 Kcal/mol
E(PM7) = 108.94007 Kcal/mol
E(ωB97X-V/def2-TZVP) = -2730.723381385006 Hartree
E(GFN1-xTB) = -120.618004568258 Hartree
E(GFN2-xTB) = -119.811483928371 Hartree
E(GFN-FF) = -16.979962862299 Hartree

Coordinates:

V	-0.137933	-0.071176	0.152538
O	1.417017	-1.148629	-0.734736
N	-0.781529	-1.204491	1.597885
N	1.079446	1.382368	0.707862
N	-1.355697	0.103107	-1.369455
C	-2.588101	0.752462	-1.208206
C	-3.289802	1.387666	-2.265222
C	-4.493929	2.060990	-2.018953
C	-5.041892	2.123008	-0.727229
C	-4.375826	1.464273	0.320492
C	-3.180271	0.778291	0.083979
C	-0.727732	0.066213	-2.639516
C	-0.436828	-1.177502	-3.245536
C	0.281506	-1.236031	-4.448341
C	0.711056	-0.055085	-5.078011
C	0.410783	1.187292	-4.492983
C	-0.300339	1.251933	-3.286477
C	2.323152	1.220980	1.315629
C	3.308057	2.240174	1.417478
C	4.540911	1.984591	2.033060
C	4.837703	0.722422	2.572138
C	3.853927	-0.281150	2.519825
C	2.615591	-0.036312	1.919038
C	0.670770	2.558819	0.044647
C	-0.645437	3.029563	0.280211
C	-1.184493	4.077961	-0.477539
C	-0.401224	4.721317	-1.449126
C	0.920898	4.291048	-1.665962
C	1.451017	3.214067	-0.944608
C	-0.876971	-2.593058	1.356168
C	-0.348385	-3.533849	2.274993
C	-0.347193	-4.899800	1.967990
C	-0.875135	-5.359598	0.746690
C	-1.425607	-4.436712	-0.156175
C	-1.438262	-3.066256	0.147244
C	-1.336956	-0.679454	2.784192
C	-2.423092	-1.316976	3.437797
C	-3.009812	-0.742121	4.571921
C	-2.543592	0.481441	5.081167
C	-1.468686	1.119194	4.440792
C	-0.864062	0.548080	3.313793
C	2.428754	-0.457214	-1.538164
C	3.297957	-1.573662	-2.099481

C	3.254167	-2.609116	-0.968118
C	1.798276	-2.541085	-0.527180
H	-2.884466	1.353766	-3.285555
H	-5.013866	2.547253	-2.859413
H	-5.984815	2.658881	-0.543722
H	-4.795631	1.467235	1.338376
H	-2.703037	0.228469	0.908826
H	-0.772476	-2.097265	-2.744544
H	0.502085	-2.214332	-4.903425
H	1.274467	-0.102998	-6.021963
H	0.745368	2.119744	-4.973468
H	-0.514027	2.222385	-2.816271
H	3.096274	3.242489	1.021574
H	5.283513	2.795616	2.094513
H	5.810093	0.530835	3.048955
H	4.044252	-1.265639	2.975688
H	1.828834	-0.807259	1.934520
H	-1.246835	2.553298	1.069586
H	-2.223934	4.391618	-0.298752
H	-0.816828	5.553942	-2.035866
H	1.540092	4.784472	-2.431314
H	2.464033	2.848749	-1.164777
H	0.072812	-3.169600	3.224224
H	0.078595	-5.616925	2.686970
H	-0.868172	-6.434012	0.509762
H	-1.865519	-4.786013	-1.103365
H	-1.883800	-2.331788	-0.541450
H	-2.809801	-2.264800	3.036323
H	-3.853737	-1.255468	5.058734
H	-3.011263	0.930565	5.969815
H	-1.080659	2.072996	4.830448
H	-0.010695	1.044618	2.829862
H	1.902348	0.140870	-2.305238
H	2.998971	0.210350	-0.860146
H	2.849484	-1.982570	-3.027912
H	4.321057	-1.220891	-2.332526
H	3.542932	-3.628649	-1.288729
H	3.920039	-2.299700	-0.136075
H	1.631203	-2.792904	0.536612
H	1.130907	-3.175327	-1.146792

Conformation 18.
Multiplicity: 3
Charge: 0
E(B97-3c) = -2729.962431448459 Hartree
E(M06/def2-TZVP) = -2729.933890158355 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -2728.974976017402 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -2729.121676073942 Hartree
E(PBEh-3c) = -2726.109735138993 Hartree
E(PM6) = 95.03061 Kcal/mol
E(PM7) = 106.83274 Kcal/mol
E(ωB97X-V/def2-TZVP) = -2730.722727107324 Hartree
E(GFN1-xTB) = -120.618089184468 Hartree
E(GFN2-xTB) = -119.807817577605 Hartree
E(GFN-FF) = -16.971498364356 Hartree

Coordinates:

V	-0.012522	0.061355	-0.244565
O	-0.407392	1.356650	1.400977
N	0.213265	1.416040	-1.662973
N	1.364834	-0.828554	0.863039
N	-1.623500	-1.037301	-0.406396
C	-1.669136	-2.384907	-0.802962
C	-2.835022	-2.966303	-1.366297
C	-2.827977	-4.297216	-1.801845
C	-1.667787	-5.083538	-1.701976
C	-0.507995	-4.515704	-1.148633
C	-0.505583	-3.190877	-0.697226
C	-2.824074	-0.352444	-0.116279
C	-3.098383	0.877821	-0.758260
C	-4.217799	1.641904	-0.390921
C	-5.096638	1.179085	0.600522
C	-4.851721	-0.062913	1.217813
C	-3.730403	-0.823517	0.867065
C	2.642836	-1.128260	0.335604
C	3.166157	-2.444045	0.405325
C	4.418680	-2.741872	-0.142373
C	5.177893	-1.739351	-0.772550
C	4.670534	-0.434197	-0.840897
C	3.420393	-0.126892	-0.284213
C	1.134881	-1.142984	2.213257
C	-0.163580	-1.508837	2.651179
C	-0.432389	-1.723584	4.008815
C	0.586489	-1.601848	4.968947
C	1.886662	-1.275226	4.543616
C	2.163361	-1.050411	3.189091
C	-0.171142	2.731517	-1.934673
C	-0.812658	3.506092	-0.931893
C	-1.261351	4.804858	-1.196542
C	-1.095860	5.379164	-2.467766
C	-0.486871	4.615046	-3.476711
C	-0.035817	3.313721	-3.224269
C	1.061395	0.681862	-2.508120
C	2.274356	1.180914	-3.059003
C	3.147880	0.318714	-3.723773
C	2.876240	-1.062050	-3.825913
C	1.684166	-1.565978	-3.296457
C	0.762901	-0.697174	-2.683579
C	0.728899	2.067567	1.978883
C	0.350819	2.266049	3.439162
C	-1.165033	2.486769	3.343250
C	-1.583349	1.494680	2.261332
H	-3.744199	-2.357112	-1.471497
H	-3.744728	-4.722917	-2.239050
H	-1.668866	-6.126991	-2.050349
H	0.411340	-5.114539	-1.053671
H	0.396826	-2.754590	-0.245173
H	-2.416401	1.224042	-1.547997
H	-4.399907	2.604373	-0.893187
H	-5.976349	1.774957	0.886542
H	-5.540710	-0.436875	1.991138
H	-3.532321	-1.788984	1.356974
H	2.571047	-3.226088	0.900922
H	4.806213	-3.770838	-0.082952
H	6.161513	-1.976978	-1.204599
H	5.254385	0.361469	-1.328008
H	3.030039	0.901160	-0.324732
H	-0.951795	-1.631932	1.893730
H	-1.450753	-2.008359	4.317251
H	0.375361	-1.777259	6.034260
H	2.699909	-1.186644	5.281041
H	3.182231	-0.787230	2.868274
H	-0.972531	3.052113	0.052615
H	-1.754521	5.375511	-0.393746
H	-1.447156	6.401079	-2.672943
H	-0.367973	5.034266	-4.488180
H	0.409558	2.725694	-4.038859
H	2.528328	2.242980	-2.931303
H	4.082772	0.720934	-4.144684
H	3.593196	-1.731468	-4.322863
H	1.435669	-2.634650	-3.381143
H	-0.236081	-1.066847	-2.398898
H	1.626703	1.441310	1.822938
H	0.846250	3.029092	1.431509
H	0.580942	1.348305	4.018662
H	0.889726	3.117052	3.898811
H	-1.693869	2.296924	4.297112
H	-1.388491	3.527505	3.028854
H	-2.430815	1.833289	1.636528
H	-1.813203	0.494422	2.675862

Conformation 23.
Multiplicity: 3
Charge: 0
E(B97-3c) = -2729.963443487621 Hartree
E(M06/def2-TZVP) = -2729.934780274221 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -2728.975572919945 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -2729.122143913105 Hartree
E(PBEh-3c) = -2726.112754512889 Hartree
E(PM6) = 100.67900 Kcal/mol
E(PM7) = 104.96765 Kcal/mol
E(ωB97X-V/def2-TZVP) = -2730.723799723231 Hartree
E(GFN1-xTB) = -120.618239351420 Hartree
E(GFN2-xTB) = -119.808564111014 Hartree
E(GFN-FF) = -16.862550004130 Hartree

Coordinates:

V	0.084955	-0.244491	0.119729
O	-0.494056	0.328922	-1.845312
N	-0.212990	1.608821	0.712793
N	-1.209830	-1.674573	0.404704
N	1.957445	-0.763471	-0.176730
C	2.973182	-0.615769	0.782314
C	4.088901	-1.490840	0.845570
C	5.042992	-1.357149	1.862147
C	4.914764	-0.361176	2.845189
C	3.813927	0.510216	2.790310
C	2.860340	0.393752	1.772476
C	2.230693	-1.427439	-1.390253
C	3.296076	-1.027555	-2.236432
C	3.469285	-1.625654	-3.489903
C	2.591579	-2.634420	-3.931393
C	1.549361	-3.054497	-3.090669
C	1.377339	-2.469245	-1.826262
C	-2.176233	-2.416664	-0.269194
C	-2.238668	-2.354566	-1.688628
C	-3.177079	-3.106823	-2.403526
C	-4.077365	-3.955605	-1.737820
C	-4.002187	-4.052584	-0.338661
C	-3.069121	-3.304150	0.389699
C	-1.102284	-1.594729	1.806553
C	-2.179391	-1.256736	2.675452

C	-1.941761	-1.022031	4.028631
C	-0.634098	-1.074814	4.558687
C	0.434310	-1.406426	3.722310
C	0.203188	-1.699037	2.363626
C	0.212629	2.717870	-0.028845
C	1.368096	2.610669	-0.850218
C	1.771986	3.669969	-1.669927
C	1.060604	4.883361	-1.679620
C	-0.056091	5.018778	-0.838156
C	-0.478299	3.960524	-0.022182
C	-1.072308	1.854622	1.821399
C	-2.475899	1.765263	1.686486
C	-3.319379	2.038867	2.772829
C	-2.775106	2.396418	4.015983
C	-1.380720	2.476205	4.164357
C	-0.536267	2.213647	3.076835
C	-1.795195	0.976095	-1.977732
C	-1.966054	1.196470	-3.474684
C	-0.521212	1.466613	-3.915787
C	0.264919	0.458108	-3.088448
H	4.191293	-2.288074	0.095230
H	5.896363	-2.052622	1.892023
H	5.666908	-0.263575	3.642029
H	3.700099	1.303359	3.545937
H	2.004872	1.084439	1.721490
H	3.973032	-0.227978	-1.899131
H	4.294785	-1.293881	-4.138846
H	2.730595	-3.096279	-4.920308
H	0.864110	-3.854705	-3.410289
H	0.578805	-2.813816	-1.152256
H	-1.511149	-1.724736	-2.216301
H	-3.196564	-3.035179	-3.502596
H	-4.815358	-4.544700	-2.301742
H	-4.680161	-4.731599	0.201938
H	-3.014773	-3.416951	1.481333
H	-3.192356	-1.155048	2.263158
H	-2.784226	-0.753391	4.683511
H	-0.462410	-0.857988	5.623317
H	1.460665	-1.468852	4.113801
H	1.020503	-2.077626	1.732922
H	1.952422	1.678613	-0.812456
H	2.672447	3.553329	-2.293627
H	1.386360	5.718809	-2.316726
H	-0.614830	5.967701	-0.815953
H	-1.356823	4.084489	0.627132
H	-2.898028	1.482182	0.711417
H	-4.410841	1.968819	2.646723
H	-3.436014	2.609723	4.869694
H	-0.944867	2.746635	5.138412
H	0.555961	2.282227	3.185502
H	-2.550425	0.301154	-1.527515
H	-1.763247	1.935843	-1.421167
H	-2.364076	0.281117	-3.960574
H	-2.656965	2.033219	-3.693384
H	-0.358470	1.328738	-5.002126
H	-0.219436	2.499160	-3.642454
H	1.287232	0.787312	-2.834424
H	0.319588	-0.544615	-3.561387

Conformation 24.
Multiplicity: 3
Charge: 0
E(B97-3c) = -2729.959646467439 Hartree
E(M06/def2-TZVP) = -2729.925289336170 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -2728.970647530242 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -2729.117039345907 Hartree
E(PBEh-3c) = -2726.107983531869 Hartree
E(PM6) = 98.70431 Kcal/mol
E(PM7) = 108.63642 Kcal/mol
E(ωB97X-V/def2-TZVP) = -2730.718292643711 Hartree
E(GFN1-xTB) = -120.618526462890 Hartree
E(GFN2-xTB) = -119.807159859993 Hartree
E(GFN-FF) = -16.972082654530 Hartree

Coordinates:

V	-0.035653	-0.059492	0.043668
O	-1.997416	0.303335	-0.529781
N	-0.046809	-1.585194	1.215163
N	0.570884	-0.393892	-1.801395
N	0.343647	1.550030	1.131214
C	1.135881	2.463102	0.405458
C	2.350306	2.017315	-0.173117
C	3.073518	2.839584	-1.048388
C	2.627620	4.138700	-1.337260
C	1.443821	4.607312	-0.739733
C	0.700475	3.783924	0.114948
C	-0.241133	1.894934	2.349974
C	-1.254726	1.063193	2.902805
C	-1.843346	1.358509	4.137738
C	-1.441661	2.484971	4.874009
C	-0.422230	3.300513	4.353414
C	0.173035	3.016855	3.118845
C	1.556377	-1.385810	-2.020705
C	1.348240	-2.718926	-1.596645
C	2.360658	-3.678780	-1.737752
C	3.589896	-3.335779	-2.322893
C	3.797799	-2.018469	-2.769323
C	2.795178	-1.051679	-2.621987
C	0.141117	0.355507	-2.905473
C	-0.215737	1.719218	-2.754114
C	-0.756111	2.446940	-3.823166
C	-0.934440	1.846844	-5.080355
C	-0.548268	0.504998	-5.254092
C	-0.016941	-0.232838	-4.190025
C	-0.965838	-2.633046	1.377718
C	-0.522121	-3.957198	1.628114
C	-1.441197	-5.005844	1.752099
C	-2.821464	-4.769343	1.631310
C	-3.271978	-3.460033	1.396314
C	-2.360094	-2.402708	1.277673
C	1.116280	-1.551720	2.023536
C	1.015346	-1.593386	3.436524
C	2.152336	-1.415890	4.230381
C	3.410194	-1.186700	3.640904
C	3.522270	-1.160867	2.244039
C	2.389786	-1.359532	1.437351
C	-2.674904	1.569488	-0.253054
C	-4.046258	1.413050	-0.897104
C	-3.733934	0.538995	-2.121016
C	-2.711950	-0.446529	-1.568330
H	2.717130	1.012249	0.080937
H	4.005515	2.462231	-1.496734
H	3.198917	4.785326	-2.019466
H	1.084069	5.625028	-0.957638
H	-0.239480	4.147004	0.556666
H	-1.546080	0.150260	2.362620
H	-2.622283	0.687672	4.533122
H	-1.903480	2.715366	5.845286
H	-0.072975	4.174848	4.925001
H	0.984640	3.656851	2.745356
H	0.384809	-2.986332	-1.138591
H	2.180656	-4.707851	-1.390615
H	4.382812	-4.090503	-2.433314
H	4.758712	-1.738821	-3.228731
H	2.957246	-0.015177	-2.954320
H	-0.021283	2.220925	-1.796104
H	-1.013098	3.507379	-3.673005
H	-1.349452	2.421305	-5.921753
H	-0.669818	0.021831	-6.236315
H	0.271022	-1.285116	-4.332227
H	0.558045	-4.145399	1.717320
H	-1.073044	-6.026319	1.940928
H	-3.539468	-5.596940	1.729177
H	-4.351323	-3.253861	1.322636
H	-2.713377	-1.372775	1.128717
H	0.026809	-1.741204	3.894792
H	2.054898	-1.436177	5.326765
H	4.298295	-1.036154	4.272615
H	4.502320	-1.004282	1.767909
H	2.492247	-1.403078	0.342924
H	-2.686488	1.714032	0.844686
H	-2.084723	2.384433	-0.722129
H	-4.742844	0.891443	-0.207842
H	-4.493753	2.391064	-1.159341
H	-4.625188	0.027345	-2.532610
H	-3.274737	1.145934	-2.927308
H	-1.967878	-0.789150	-2.309327
H	-3.177826	-1.327049	-1.077577

Conformation 25.
Multiplicity: 3
Charge: 0
E(B97-3c) = -2729.955983537547 Hartree
E(M06/def2-TZVP) = -2729.925799006199 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -2728.967883495028 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -2729.113726898050 Hartree
E(PBEh-3c) = -2726.103006289170 Hartree
E(PM6) = 101.67079 Kcal/mol
E(PM7) = 106.53882 Kcal/mol
E(ωB97X-V/def2-TZVP) = -2730.714756718114 Hartree
E(GFN1-xTB) = -120.617452474203 Hartree
E(GFN2-xTB) = -119.807681266316 Hartree
E(GFN-FF) = -16.864314400124 Hartree

Coordinates:

V	0.074114	0.117593	-0.072313
O	-1.546208	0.058277	-1.435743
N	-0.134847	-1.624383	0.781188
N	1.309470	0.617901	-1.608712
N	-0.387592	1.505243	1.157273
C	0.636731	1.195669	2.080296
C	1.979104	1.172811	1.617747

C	2.996269	0.632685	2.429223
C	2.704231	0.158286	3.709622
C	1.378520	0.223109	4.190506
C	0.353790	0.729943	3.394052
C	-1.462299	2.339095	1.472340
C	-1.333536	3.373931	2.433787
C	-2.409175	4.226967	2.708197
C	-3.635127	4.079297	2.037725
C	-3.770956	3.056933	1.084024
C	-2.704442	2.194467	0.803477
C	1.970475	-0.516647	-2.102505
C	1.223818	-1.678443	-2.430122
C	1.864112	-2.877774	-2.775160
C	3.263329	-2.943508	-2.839968
C	4.017501	-1.790115	-2.549783
C	3.388091	-0.596677	-2.181853
C	1.591098	1.887996	-2.106104
C	2.246238	2.091910	-3.355352
C	2.469643	3.380987	-3.851750
C	2.045634	4.518215	-3.142380
C	1.380427	4.333412	-1.919406
C	1.155377	3.050334	-1.406567
C	-1.438324	-2.126789	0.989781
C	-2.453333	-1.303300	1.529258
C	-3.772003	-1.773275	1.643183
C	-4.097294	-3.078210	1.243418
C	-3.085290	-3.918532	0.739946
C	-1.770874	-3.453764	0.618346
C	0.925442	-2.265358	1.452270
C	0.722858	-2.917357	2.697552
C	1.793530	-3.506418	3.379012
C	3.094549	-3.460124	2.849153
C	3.303799	-2.823648	1.615647
C	2.237859	-2.240219	0.920373
C	-1.625365	1.146409	-2.409932
C	-2.977331	0.952565	-3.078387
C	-3.082378	-0.578350	-3.122537
C	-2.516490	-0.986255	-1.765996
H	2.223609	1.615295	0.640363
H	4.026851	0.597759	2.046037
H	3.498059	-0.270663	4.337638
H	1.144921	-0.155321	5.197406
H	-0.685706	0.746394	3.752982
H	-0.373830	3.503314	2.955159
H	-2.284256	5.025468	3.455993
H	-4.475987	4.753332	2.257712
H	-4.727000	2.920406	0.554640
H	-2.818200	1.378012	0.078321
H	0.126639	-1.625825	-2.399532
H	1.258388	-3.768092	-3.004348
H	3.765971	-3.883090	-3.112433
H	5.117262	-1.829603	-2.592402
H	3.983544	0.291830	-1.924963
H	2.570960	1.220078	-3.940985
H	2.979407	3.496971	-4.821526
H	2.224740	5.528058	-3.539557
H	1.028242	5.204228	-1.344304
H	0.625538	2.929153	-0.450077
H	-2.191717	-0.288940	1.860120
H	-4.546563	-1.109825	2.058174
H	-5.129815	-3.447447	1.334418
H	-3.328643	-4.947386	0.431980
H	-0.976950	-4.101566	0.216832
H	-0.287766	-2.942589	3.129786
H	1.609605	-4.000721	4.345877
H	3.933119	-3.925792	3.388340
H	4.310936	-2.788913	1.171958
H	2.419406	-1.773865	-0.055573
H	-1.508656	2.100324	-1.859169
H	-0.779064	1.045248	-3.119661
H	-3.788021	1.385757	-2.455584
H	-3.019017	1.427735	-4.077129
H	-4.115864	-0.948206	-3.266150
H	-2.456102	-0.981764	-3.945021
H	-1.993049	-1.961080	-1.761435
H	-3.284136	-1.003563	-0.966717

Conformation 26.
Multiplicity: 3
Charge: 0
E(B97-3c) = -2729.964216386315 Hartree
E(M06/def2-TZVP) = -2729.930975643906 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -2728.974510974628 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -2729.122015287553 Hartree
E(PBEh-3c) = -2726.114188423216 Hartree
E(PM6) = 97.21117 Kcal/mol
E(PM7) = 108.99983 Kcal/mol
E(ωB97X-V/def2-TZVP) = -2730.723269768401 Hartree
E(GFN1-xTB) = -120.617648913205 Hartree
E(GFN2-xTB) = -119.810159717639 Hartree
E(GFN-FF) = -16.977859831628 Hartree

Coordinates:

V	-0.197347	-0.051908	0.003607
O	1.358489	-0.789359	1.191465
N	-1.823320	-0.608040	0.916008
N	0.193916	1.857244	0.138218
N	0.313021	-1.139769	-1.559348
C	0.586148	-0.228895	-2.601915
C	1.876465	-0.038888	-3.164024
C	2.103513	0.997875	-4.077522
C	1.069545	1.884115	-4.432872
C	-0.209757	1.706033	-3.884853
C	-0.456332	0.644183	-3.003563
C	0.704382	-2.477194	-1.564076
C	0.392133	-3.271596	-0.423820
C	0.777365	-4.613469	-0.348835
C	1.461434	-5.225055	-1.414398
C	1.726335	-4.468372	-2.567363
C	1.354883	-3.119758	-2.651619
C	1.542820	2.182279	0.432268
C	1.975041	2.234980	1.777166
C	3.325571	2.452217	2.085803
C	4.267411	2.640089	1.058770
C	3.843704	2.608926	-0.280802
C	2.495988	2.380342	-0.595341
C	-0.643162	2.804299	-0.467530
C	-0.202972	4.082459	-0.898263
C	-1.083459	4.959879	-1.544842
C	-2.422163	4.605029	-1.779561
C	-2.879199	3.356527	-1.323812
C	-2.012679	2.476917	-0.666538
C	-3.020821	-0.906582	0.233300
C	-4.286863	-0.564005	0.775541
C	-5.461791	-0.808386	0.053526
C	-5.413041	-1.389206	-1.224586
C	-4.164415	-1.734270	-1.767731
C	-2.983054	-1.507526	-1.050794
C	-1.865113	-0.479650	2.324689
C	-2.226264	-1.576992	3.143192
C	-2.161553	-1.472984	4.538010
C	-1.744889	-0.274310	5.146796
C	-1.414339	0.828152	4.343201
C	-1.483082	0.733122	2.943865
C	1.285401	-1.289921	2.559418
C	2.733062	-1.559307	2.951510
C	3.365432	-1.956701	1.611479
C	2.707087	-0.977532	0.651169
H	2.707167	-0.686620	-2.849503
H	3.111628	1.133992	-4.499331
H	1.263508	2.708761	-5.134613
H	-1.028853	2.393819	-4.143050
H	-1.470194	0.478086	-2.607224
H	-0.191989	-2.816574	0.391806
H	0.518184	-5.197381	0.548404
H	1.760164	-6.281912	-1.356227
H	2.230361	-4.936935	-3.427188
H	1.556882	-2.556633	-3.572660
H	1.232031	2.084007	2.574052
H	3.645491	2.482755	3.139155
H	5.326534	2.812740	1.302184
H	4.572721	2.751330	-1.093541
H	2.165909	2.329867	-1.643272
H	0.839413	4.384720	-0.728835
H	-0.711000	5.943254	-1.872516
H	-3.104358	5.299355	-2.291861
H	-3.930826	3.062349	-1.464701
H	-2.403040	1.524526	-0.277092
H	-4.335726	-0.091752	1.767279
H	-6.431396	-0.529737	0.495038
H	-6.338805	-1.575202	-1.788897
H	-4.105008	-2.202685	-2.762317
H	-2.009990	-1.799675	-1.470835
H	-2.543723	-2.514207	2.661406
H	-2.432303	-2.339899	5.160560
H	-1.691725	-0.199298	6.243222
H	-1.110844	1.779311	4.807700
H	-1.234904	1.591310	2.301509
H	0.776200	-0.530091	3.180340
H	0.671440	-2.215000	2.553643
H	3.204336	-0.633111	3.340167
H	2.811942	-2.343396	3.728976
H	4.468780	-1.867556	1.602883
H	3.092754	-2.997484	1.339774
H	2.605757	-1.360703	-0.380118
H	3.209948	0.010679	0.640691

Conformation 3.
Multiplicity: 3
Charge: 0
E(B97-3c) = -2729.966391890795 Hartree
E(M06/def2-TZVP) = -2729.935869948631 Hartree

E(PBE - D3(BJ)/def2-TZVP) = -2728.978110775809 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -2729.125807407539 Hartree
E(PBEh-3c) = -2726.115001053493 Hartree
E(PM6) = 93.45212 Kcal/mol
E(PM7) = 107.94963 Kcal/mol
E(ωB97X-V/def2-TZVP) = -2730.727558605072 Hartree
E(GFN1-xTB) = -120.620694896015 Hartree
E(GFN2-xTB) = -119.811519704521 Hartree
E(GFN-FF) = -16.974265006480 Hartree

Coordinates:

V	0.127535	0.008650	-0.008529
O	-1.232230	-0.840392	-1.376001
N	1.551582	-1.322939	-0.143080
N	0.205770	1.694905	-1.045249
N	-0.880349	0.056511	1.660524
C	-0.620298	0.995508	2.673029
C	-0.731751	0.663771	4.047177
C	-0.391710	1.595634	5.035375
C	0.072222	2.876213	4.689770
C	0.180301	3.216224	3.330701
C	-0.169422	2.297536	2.334178
C	-1.729648	-1.038556	1.922004
C	-3.084289	-0.852391	2.292552
C	-3.942977	-1.951141	2.415195
C	-3.473214	-3.257398	2.179112
C	-2.124254	-3.454754	1.845014
C	-1.254119	-2.358309	1.732957
C	1.424329	2.366613	-1.279657
C	2.590672	1.636677	-1.616068
C	3.823168	2.286635	-1.770496
C	3.920498	3.678015	-1.615934
C	2.765660	4.414725	-1.298034
C	1.533581	3.772875	-1.127741
C	-0.978876	2.251921	-1.558546
C	-1.023550	2.867528	-2.837940
C	-2.236535	3.317214	-3.373413
C	-3.438814	3.170407	-2.657280
C	-3.403743	2.582733	-1.382235
C	-2.192389	2.139912	-0.833202
C	2.296609	-1.088855	1.022234
C	2.386130	0.250192	1.487961
C	2.875805	0.537757	2.771533
C	3.362300	-0.494100	3.583935
C	3.339375	-1.819647	3.104849
C	2.804876	-2.125515	1.849852
C	1.787689	-2.464281	-0.928617
C	3.099384	-2.777754	-1.364880
C	3.334616	-3.892741	-2.178036
C	2.272707	-4.722184	-2.579084
C	0.971409	-4.426805	-2.142944
C	0.728210	-3.317067	-1.320587
C	-2.640825	-1.187932	-1.195276
C	-3.153479	-1.500850	-2.599033
C	-2.252431	-0.636825	-3.492379
C	-0.905099	-0.770848	-2.799283
H	-1.068243	-0.344065	4.329898
H	-0.479327	1.310201	6.095425
H	0.342312	3.601948	5.471192
H	0.532554	4.217236	3.036672
H	-0.091618	2.575560	1.272599
H	-3.452280	0.171038	2.460990
H	-4.997188	-1.788248	2.688450
H	-4.155224	-4.115958	2.270609
H	-1.736196	-4.472098	1.681969
H	-0.188455	-2.505402	1.503140
H	2.513369	0.545654	-1.744046
H	4.715962	1.694779	-2.024758
H	4.887595	4.186877	-1.742546
H	2.828205	5.506506	-1.168577
H	0.634871	4.351949	-0.867558
H	-0.090666	2.976851	-3.410967
H	-2.245307	3.782157	-4.371718
H	-4.388598	3.525640	-3.083759
H	-4.329891	2.482380	-0.794731
H	-2.162512	1.699898	0.175964
H	2.111785	1.085591	0.817683
H	2.885318	1.580589	3.121536
H	3.764873	-0.272116	4.583016
H	3.726030	-2.634705	3.736673
H	2.749275	-3.167345	1.501804
H	3.929739	-2.124928	-1.055813
H	4.360961	-4.113313	-2.510336
H	2.460583	-5.595430	-3.221307
H	0.132105	-5.077780	-2.434198
H	-0.285031	-3.098428	-0.956609
H	-2.699975	-2.037767	-0.489549
H	-3.148714	-0.310007	-0.750050
H	-3.019835	-2.577305	-2.833671
H	-4.228860	-1.259590	-2.703589
H	-2.216629	-0.984992	-4.542785
H	-2.584306	0.421441	-3.483250
H	-0.229657	0.093132	-2.940167
H	-0.371451	-1.706822	-3.072063

Conformation 31.
Multiplicity: 3
Charge: 0
E(B97-3c) = -2729.958255893322 Hartree
E(M06/def2-TZVP) = -2729.925008681189 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -2728.968740555135 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -2729.112489313793 Hartree
E(PBEh-3c) = -2726.102786504222 Hartree
E(PM6) = 96.24529 Kcal/mol
E(PM7) = 111.94988 Kcal/mol
E(ωB97X-V/def2-TZVP) = -2730.713056956968 Hartree
E(GFN1-xTB) = -120.623932761891 Hartree
E(GFN2-xTB) = -119.809801963980 Hartree
E(GFN-FF) = -16.965474518106 Hartree

Coordinates:

V	0.072688	0.203866	-0.350068
O	2.167481	0.633990	-0.916409
N	-1.671638	0.330633	-1.204207
N	0.492721	-1.708377	-0.226716
N	-0.034411	1.166958	1.338637
C	-0.826777	0.730297	2.419543
C	-1.040424	-0.651879	2.649153
C	-1.881062	-1.086460	3.681717
C	-2.519891	-0.161594	4.523275
C	-2.301754	1.210942	4.315438
C	-1.469810	1.655924	3.280873
C	0.687333	2.372185	1.485452
C	1.565779	2.567741	2.582263
C	2.361298	3.716169	2.662347
C	2.301858	4.700142	1.657012
C	1.416094	4.527959	0.581831
C	0.605949	3.384779	0.501686
C	1.685790	-2.147824	0.378966
C	2.270813	-1.415667	1.443018
C	3.512636	-1.786986	1.975445
C	4.200746	-2.906074	1.478036
C	3.616517	-3.658640	0.443011
C	2.378789	-3.292029	-0.099312
C	-0.403361	-2.703843	-0.691689
C	-0.829278	-3.750041	0.162433
C	-1.782576	-4.679066	-0.270814
C	-2.328906	-4.589521	-1.562530
C	-1.894679	-3.571011	-2.424404
C	-0.932896	-2.645581	-1.999124
C	-1.581314	1.595628	-1.806917
C	-2.497551	2.647426	-1.527573
C	-2.259438	3.935217	-2.010226
C	-1.108825	4.221532	-2.777536
C	-0.212775	3.190967	-3.085355
C	-0.457715	1.883180	-2.627551
C	-2.896037	-0.354038	-1.187126
C	-3.227991	-1.188925	-0.096445
C	-4.398993	-1.953045	-0.117572
C	-5.278715	-1.886554	-1.211365
C	-4.968662	-1.040649	-2.289111
C	-3.790585	-0.282801	-2.283642
C	2.718607	-0.126568	-2.023629
C	4.185603	-0.321357	-1.669605
C	4.518810	1.016499	-0.995132
C	3.243452	1.336158	-0.214191
H	-0.533065	-1.380404	2.001916
H	-2.029596	-2.167127	3.832887
H	-3.177818	-0.505453	5.335196
H	-2.796893	1.950953	4.963576
H	-1.317984	2.732868	3.117417
H	1.618956	1.794401	3.363619
H	3.044626	3.843689	3.516500
H	2.932168	5.599618	1.722760
H	1.335892	5.297481	-0.201667
H	-0.108893	3.274481	-0.323682
H	1.725802	-0.550465	1.849019
H	3.938860	-1.199682	2.804051
H	5.172277	-3.199884	1.902330
H	4.136787	-4.544728	0.046668
H	1.932176	-3.882001	-0.913188
H	-0.409719	-3.812830	1.178053
H	-2.114436	-5.475022	0.413884
H	-3.090745	-5.310291	-1.894645
H	-2.314988	-3.488119	-3.437964
H	-0.602158	-1.837105	-2.667649
H	-3.374919	2.430142	-0.901137
H	-2.968006	4.742678	-1.769044
H	-0.928003	5.243593	-3.142087
H	0.672924	3.392663	-3.707168
H	0.193442	1.051411	-2.940495
H	-2.551026	-1.224135	0.766787

H	-4.629123	-2.604715	0.739213
H	-6.201093	-2.486412	-1.222767
H	-5.647923	-0.977654	-3.153780
H	-3.538671	0.358158	-3.142012
H	2.137652	-1.066001	-2.101875
H	2.594009	0.464263	-2.960436
H	4.294539	-1.164202	-0.957079
H	4.809918	-0.532349	-2.559526
H	5.401944	0.957250	-0.329966
H	4.719257	1.798062	-1.757295
H	2.992101	2.412981	-0.182705
H	3.274827	0.944224	0.820408

Conformation 33.
Multiplicity: 3
Charge: 0
E(B97-3c) = -2729.966379523576 Hartree
E(M06/def2-TZVP) = -2729.934747889639 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -2728.976862559467 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -2729.125272920965 Hartree
E(PBEh-3c) = -2726.116737702291 Hartree
E(PM6) = 93.19738 Kcal/mol
E(PM7) = 113.51464 Kcal/mol
E(ωB97X-V/def2-TZVP) = -2730.727523297464 Hartree
E(GFN1-xTB) = -120.620439160570 Hartree
E(GFN2-xTB) = -119.810560363668 Hartree
E(GFN-FF) = -16.973760565180 Hartree

Coordinates:

V	0.046472	-0.065751	-0.042627
O	-1.758118	0.631859	0.737896
N	0.605700	1.727397	-0.635731
N	1.067179	-0.809936	1.438999
N	-0.722648	-1.369695	-1.270465
C	0.170037	-2.244425	-1.903495
C	1.562349	-1.982400	-1.809542
C	2.503651	-2.862651	-2.350832
C	2.084908	-4.019442	-3.030652
C	0.709566	-4.280358	-3.148685
C	-0.241061	-3.413494	-2.592570
C	-2.100801	-1.415687	-1.592421
C	-2.558937	-1.025659	-2.873006
C	-3.929662	-0.989781	-3.161766
C	-4.872122	-1.345502	-2.181000
C	-4.426432	-1.755593	-0.913554
C	-3.054671	-1.801122	-0.623410
C	2.470625	-0.878102	1.470602
C	3.244046	0.052066	0.727566
C	4.639518	-0.048211	0.685154
C	5.308702	-1.056479	1.398839
C	4.553332	-1.967505	2.155894
C	3.155438	-1.889573	2.191791
C	0.316809	-1.449804	2.451325
C	0.378589	-1.014654	3.797375
C	-0.469389	-1.572362	4.762232
C	-1.389348	-2.577655	4.409168
C	-1.433058	-3.039676	3.084077
C	-0.577982	-2.491646	2.114331
C	0.380052	2.830023	0.208848
C	-0.051160	4.083452	-0.297885
C	-0.380523	5.129469	0.572618
C	-0.289914	4.960195	1.966845
C	0.156214	3.730764	2.478413
C	0.497925	2.681705	1.613045
C	1.342860	1.901123	-1.822789
C	1.054098	1.102380	-2.956118
C	1.846557	1.177397	-4.109079
C	2.929509	2.067684	-4.173349
C	3.213359	2.880864	-3.061682
C	2.439970	2.798964	-1.897899
C	-2.601073	1.512391	-0.076316
C	-3.302662	2.398689	0.939763
C	-3.525560	1.415423	2.097153
C	-2.212412	0.640349	2.125669
H	1.938433	-1.067968	-1.316473
H	3.574316	-2.629116	-2.248831
H	2.823835	-4.707879	-3.466416
H	0.365995	-5.182778	-3.678416
H	-1.313958	-3.638928	-2.676001
H	-1.818801	-0.738431	-3.635256
H	-4.266825	-0.670999	-4.160191
H	-5.948411	-1.309489	-2.406971
H	-5.154888	-2.051032	-0.142227
H	-2.701718	-2.120009	0.367259
H	2.735866	0.866206	0.190601
H	5.208519	0.685044	0.092754
H	6.405919	-1.129334	1.369014
H	5.060204	-2.765006	2.721594
H	2.575842	-2.624159	2.769073
H	1.092136	-0.220528	4.065120
H	-0.420838	-1.213101	5.801962
H	-2.058797	-3.006820	5.169656
H	-2.129995	-3.844066	2.801673
H	-0.581951	-2.857073	1.076650
H	-0.133352	4.217476	-1.387079
H	-0.722248	6.090464	0.157361
H	-0.551768	5.785484	2.645543
H	0.258027	3.589409	3.565887
H	0.874197	1.724032	2.006798
H	0.189646	0.423448	-2.912911
H	1.605201	0.534881	-4.969730
H	3.547493	2.130492	-5.081274
H	4.061327	3.582715	-3.095972
H	2.682397	3.423728	-1.025434
H	-1.937186	2.046220	-0.780108
H	-3.310380	0.873294	-0.641922
H	-2.636943	3.230806	1.248724
H	-4.241796	2.828467	0.540941
H	-3.735628	1.908244	3.065902
H	-4.370900	0.734767	1.864554
H	-2.303874	-0.407305	2.469702
H	-1.439030	1.153812	2.731717

LUFCIZ

Conformation 2.
Multiplicity: 5
Charge: 0
E(B97-3c) = -3593.871077226790 Hartree
E(GFN1-xTB) = -169.715092985715 Hartree
E(GFN2-xTB) = -169.230178231737 Hartree
E(GFN-FF) = -24.136567205388 Hartree
E(M06/def2-TZVP) = -3593.616731544692 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3592.337878491573 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3592.631458288078 Hartree
E(PBEh-3c) = -3588.830996805323 Hartree
E(PM6) = 151.18855 Kcal/mol
E(PM7) = 51.26554 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3596.387030838947 Hartree

Coordinates:

Fe	-0.103815	0.531318	-0.098951
C	-1.418516	0.004414	1.354142
C	-2.163119	-1.012507	2.007383
C	-2.533755	-0.830699	3.360032
H	-3.064790	-1.645891	3.876794
C	-2.306579	0.382960	4.024428
H	-2.635499	0.508670	5.067231
C	-1.727343	1.458869	3.339293
H	-1.657034	2.439831	3.827556
C	-1.271989	1.271345	2.017006
C	-2.792504	-2.192784	1.314992
C	-2.120872	-3.426661	1.131880
C	-2.829095	-4.523539	0.600154
H	-2.309820	-5.484709	0.461991
C	-4.184453	-4.417221	0.270796
H	-4.727996	-5.286787	-0.129404
C	-4.842688	-3.193356	0.443351
H	-5.905836	-3.107913	0.170323
C	-4.166191	-2.067656	0.948806
C	-0.678797	-3.614317	1.575436
H	-0.326264	-2.626505	1.931718
C	0.240780	-4.052148	0.425323
H	0.251701	-3.301180	-0.389428
H	-0.080029	-5.021909	-0.008604
H	1.284161	-4.173141	0.777330
C	-0.619167	-4.588188	2.765750
H	-1.242020	-4.225698	3.608522
H	0.419294	-4.709499	3.134501
H	-0.991994	-5.594213	2.482459
C	-4.930787	-0.753704	1.108812
H	-4.192144	0.034976	1.355988
C	-5.637424	-0.324358	-0.187837
H	-4.930735	-0.278703	-1.039554
H	-6.093414	0.679603	-0.064827
H	-6.452323	-1.023668	-0.467178
C	-5.926554	-0.825534	2.278843
H	-5.413273	-1.064134	3.230831
H	-6.693078	-1.609178	2.104006
H	-6.454311	0.142150	2.407623
C	-0.633259	2.331007	1.160008
C	-1.165047	2.489688	-0.193189
C	-0.439249	3.316067	-1.095965
H	-0.803990	3.417054	-2.127318
C	0.692613	4.019540	-0.691625
H	1.243262	4.638941	-1.414534
C	1.107483	3.970507	0.650513
H	1.966264	4.578996	0.967491
C	0.466784	3.152543	1.591413
C	-2.629202	2.145000	-0.523700
H	-2.873722	1.181141	-0.037889

C	-3.536411	3.215443	0.109487
H	-3.393194	3.264140	1.207602
H	-4.603200	2.982818	-0.088042
H	-3.317524	4.219445	-0.310276
C	-2.905341	1.981434	-2.019513
H	-2.228882	1.239239	-2.485569
H	-2.799105	2.935046	-2.575887
H	-3.945103	1.632153	-2.175499
C	0.920157	3.195365	3.043694
H	0.628078	2.232609	3.511006
C	2.437041	3.342521	3.205013
H	2.982555	2.613624	2.581071
H	2.729253	3.171738	4.260543
H	2.787320	4.360218	2.934175
C	0.196714	4.337760	3.786368
H	-0.904970	4.287276	3.679327
H	0.515758	5.319601	3.379204
H	0.442000	4.321405	4.868260
C	1.458076	-0.350770	-0.970198
C	2.638682	-0.791302	-0.296365
C	3.371987	-1.886145	-0.805768
H	4.268283	-2.224577	-0.262012
C	2.997645	-2.516401	-2.000813
H	3.570097	-3.377966	-2.376882
C	1.938039	-1.990462	-2.749171
H	1.701839	-2.402485	-3.742613
C	1.183694	-0.901384	-2.257806
C	3.294358	-0.062850	0.852351
C	3.123367	-0.465837	2.202418
C	3.957104	0.082001	3.197780
H	3.835325	-0.243665	4.242157
C	4.948177	1.014779	2.877013
H	5.601142	1.423112	3.663558
C	5.087519	1.443463	1.551819
H	5.855030	2.191684	1.300856
C	4.270723	0.925071	0.528798
C	2.129105	-1.552792	2.578127
H	1.474825	-1.703725	1.694952
C	1.235187	-1.160676	3.762860
H	0.684487	-0.220971	3.560475
H	1.821576	-1.024316	4.694851
H	0.480715	-1.947655	3.963259
C	2.877086	-2.871017	2.844624
H	3.461015	-3.187214	1.957424
H	2.172437	-3.686928	3.100674
H	3.586165	-2.758764	3.691019
C	4.510669	1.370512	-0.909890
H	3.668979	0.982337	-1.514084
C	4.513700	2.898658	-1.062545
H	3.570450	3.338503	-0.683082
H	4.618815	3.179566	-2.130842
H	5.355998	3.371463	-0.516270
C	5.800534	0.745829	-1.468933
H	5.758722	-0.360283	-1.423096
H	6.689358	1.076928	-0.892168
H	5.953243	1.037226	-2.528776
C	0.175844	-0.285551	-3.194145
C	0.495427	0.938167	-3.866466
C	-0.380762	1.412115	-4.860161
H	-0.145359	2.346073	-5.389315
C	-1.539052	0.705347	-5.210220
H	-2.201341	1.089841	-6.001099
C	-1.853844	-0.479608	-4.542416
H	-2.774271	-1.023391	-4.803450
C	-1.017575	-0.983018	-3.525380
C	1.796806	1.686049	-3.583661
H	1.951913	1.643147	-2.484436
C	2.994121	0.987407	-4.257835
H	3.121037	-0.053707	-3.907194
H	3.935053	1.534510	-4.043110
H	2.856944	0.964728	-5.358921
C	1.775569	3.163483	-3.997657
H	0.877311	3.693879	-3.627004
H	1.803582	3.281560	-5.100856
H	2.668627	3.680613	-3.593484
C	-1.431340	-2.247741	-2.787652
H	-0.757932	-2.350540	-1.912365
C	-2.862449	-2.130579	-2.252827
H	-2.976749	-1.227326	-1.623336
H	-3.117537	-3.007017	-1.630313
H	-3.609249	-2.073087	-3.071619
C	-1.267297	-3.509868	-3.649656
H	-0.219395	-3.648592	-3.980954
H	-1.904526	-3.460334	-4.557476
H	-1.566522	-4.410162	-3.074379

Conformation 25.
Multiplicity: 5
Charge: 0
E(B97-3c) = -3593.864730263530 Hartree
E(GFN1-xTB) = -169.715152983924 Hartree
E(GFN2-xTB) = -169.236440741096 Hartree
E(GFN-FF) = -24.051237318642 Hartree
E(M06/def2-TZVP) = -3593.612440974443 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3592.328706835875 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3592.632086238828 Hartree
E(PBEh-3c) = -3588.834590178223 Hartree
E(PM6) = 175.76578 Kcal/mol
E(PM7) = 62.98373 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3596.392810185007 Hartree

Coordinates:

Fe	0.147149	0.056866	0.408117
C	1.956544	-0.213910	-0.499227
C	2.526716	-0.614680	-1.742415
C	3.879898	-0.320304	-2.025904
H	4.300777	-0.647014	-2.989352
C	4.708865	0.305040	-1.085454
H	5.765305	0.500988	-1.322871
C	4.198469	0.612069	0.179435
H	4.858324	1.016641	0.962923
C	2.839570	0.361336	0.465883
C	1.861155	-1.535451	-2.728181
C	1.251789	-1.058626	-3.919840
C	0.791050	-1.995507	-4.865132
H	0.323154	-1.642595	-5.795599
C	0.899099	-3.372338	-4.636242
H	0.519137	-4.087331	-5.382415
C	1.494898	-3.835174	-3.457853
H	1.590432	-4.918887	-3.287614
C	2.000972	-2.934911	-2.500344
C	1.117502	0.437902	-4.195596
H	1.108632	0.946597	-3.207210
C	-0.182744	0.800925	-4.929147
H	-1.080149	0.475165	-4.368992
H	-0.225044	0.347698	-5.940119
H	-0.251737	1.896346	-5.075183
C	2.333634	0.966065	-4.979396
H	3.280465	0.782091	-4.437902
H	2.246784	2.058957	-5.150117
H	2.406426	0.469889	-5.969460
C	2.782666	-3.476875	-1.305066
H	2.939062	-2.635835	-0.603018
C	2.034916	-4.572434	-0.536534
H	1.062857	-4.203679	-0.156790
H	2.635170	-4.913775	0.331795
H	1.838541	-5.465259	-1.165894
C	4.176093	-3.952567	-1.752850
H	4.742093	-3.133489	-2.238972
H	4.099913	-4.788351	-2.479112
H	4.767442	-4.307660	-0.883617
C	2.328235	0.616339	1.857664
C	2.000741	-0.508904	2.686855
C	1.619184	-0.268652	4.024807
H	1.381913	-1.119584	4.676932
C	1.581658	1.025740	4.545562
H	1.280861	1.189999	5.591319
C	1.942065	2.117694	3.743265
H	1.925706	3.127192	4.174987
C	2.328237	1.942373	2.404812
C	2.244972	-1.948361	2.223625
H	1.919530	-2.016818	1.164462
C	3.752404	-2.265734	2.258298
H	4.334074	-1.578178	1.615526
H	3.933674	-3.300111	1.900768
H	4.143894	-2.186086	3.294000
C	1.459626	-3.001354	3.009161
H	0.380112	-2.767184	3.042220
H	1.828390	-3.109988	4.050324
H	1.564195	-3.988994	2.519393
C	2.739717	3.138114	1.548893
H	3.705388	2.877245	1.067729
C	1.714754	3.371699	0.432867
H	1.597930	2.480647	-0.215176
H	2.014269	4.217866	-0.216681
H	0.730364	3.613152	0.870719
C	2.960028	4.433076	2.338966
H	3.690146	4.305102	3.163453
H	2.010806	4.814569	2.769599
H	3.347872	5.223202	1.665281
C	-1.849413	0.408012	0.210194
C	-2.472750	1.670077	-0.023315
C	-3.828686	1.743406	-0.418573
H	-4.273471	2.734646	-0.597627
C	-4.616322	0.591850	-0.532315
H	-5.673543	0.667098	-0.829307
C	-4.050696	-0.649063	-0.220817
H	-4.661160	-1.565077	-0.253777
C	-2.688175	-0.743997	0.129273
C	-1.841386	2.999805	0.280288
C	-1.366693	3.847987	-0.756497
C	-1.013820	5.174381	-0.439586

H	-0.662312	5.846308	-1.236464
C	-1.080177	5.648371	0.875087
H	-0.792680	6.686341	1.103362
C	-1.497854	4.792541	1.901582
H	-1.538984	5.165836	2.935919
C	-1.897087	3.470389	1.625412
C	-1.240549	3.354710	-2.196184
H	-1.262252	2.244218	-2.160456
C	0.091073	3.777730	-2.837897
H	0.958089	3.387953	-2.271346
H	0.192026	4.880352	-2.896758
H	0.163105	3.396139	-3.873997
C	-2.432662	3.813207	-3.054357
H	-3.392374	3.455966	-2.633912
H	-2.346973	3.420326	-4.088596
H	-2.477675	4.920910	-3.111760
C	-2.469736	2.603070	2.743983
H	-2.389869	1.550149	2.407455
C	-1.697419	2.716694	4.062484
H	-0.622010	2.504234	3.914971
H	-2.088908	1.986676	4.799622
H	-1.793123	3.722595	4.521335
C	-3.964113	2.909382	2.950200
H	-4.540343	2.755556	2.017081
H	-4.109154	3.962415	3.271149
H	-4.396062	2.250576	3.732267
C	-2.186211	-2.102814	0.521647
C	-2.235190	-2.438576	1.909726
C	-1.880678	-3.738029	2.314760
H	-1.932494	-4.008072	3.380813
C	-1.480543	-4.698396	1.378489
H	-1.195578	-5.709246	1.707570
C	-1.457308	-4.368947	0.020787
H	-1.169499	-5.129485	-0.722204
C	-1.819368	-3.084617	-0.439830
C	-2.799018	-1.460420	2.938330
H	-2.895000	-0.477859	2.437211
C	-4.216019	-1.893019	3.354626
H	-4.882324	-1.974467	2.472820
H	-4.662148	-1.156602	4.054878
H	-4.205261	-2.881259	3.860271
C	-1.888785	-1.254739	4.154663
H	-0.910433	-0.830742	3.856791
H	-1.699526	-2.200488	4.704160
H	-2.356518	-0.547247	4.869475
C	-1.893713	-2.921540	-1.958165
H	-1.050065	-3.527323	-2.354763
C	-3.194933	-3.556354	-2.489701
H	-3.315237	-4.603203	-2.146569
H	-3.201382	-3.551492	-3.599304
H	-4.078580	-2.982077	-2.143428
C	-1.724032	-1.517157	-2.541821
H	-0.852644	-0.994682	-2.102435
H	-2.616129	-0.882040	-2.394114
H	-1.540572	-1.608945	-3.628152

Conformation 27.
Multiplicity: 5
Charge: 0
E(B97-3c) = -3593.855891483977 Hartree
E(GFN1-xTB) = -169.710964105228 Hartree
E(GFN2-xTB) = -169.232663529372 Hartree
E(GFN-FF) = -24.044367125238 Hartree
E(M06/def2-TZVP) = -3593.603482345096 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3592.318520362066 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3592.623967292348 Hartree
E(PBEh-3c) = -3588.825210403138 Hartree
E(PM6) = 194.26395 Kcal/mol
E(PM7) = 69.19441 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3596.391768741060 Hartree

Coordinates:

Fe	0.034229	-0.339716	0.155920
C	-2.019316	-0.332926	-0.047390
C	-2.638612	-1.270936	0.836359
C	-4.039653	-1.353540	0.984613
H	-4.456400	-2.084667	1.694125
C	-4.884806	-0.546421	0.218213
H	-5.978807	-0.620519	0.317857
C	-4.310846	0.345938	-0.690516
H	-4.953497	0.977186	-1.323088
C	-2.907459	0.482557	-0.810433
C	-1.872165	-2.320438	1.591122
C	-1.501301	-2.150888	2.954987
C	-1.019228	-3.271763	3.661692
H	-0.745440	-3.150496	4.721655
C	-0.889762	-4.522637	3.051603
H	-0.505814	-5.379496	3.626336
C	-1.238254	-4.676654	1.706246
H	-1.135547	-5.661346	1.226710
C	-1.743318	-3.596545	0.962135
C	-1.656742	-0.849838	3.745631
H	-1.041310	-1.005646	4.658404
C	-3.099650	-0.626982	4.240191
H	-3.483914	-1.520298	4.772278
H	-3.784321	-0.406102	3.398169
H	-3.136489	0.232356	4.941435
C	-1.111907	0.418104	3.071409
H	-0.118360	0.246987	2.594927
H	-0.967524	1.216916	3.824934
H	-1.794450	0.813114	2.294953
C	-2.269365	-3.839234	-0.452450
H	-2.432548	-2.848018	-0.921534
C	-1.289944	-4.608844	-1.346892
H	-0.317039	-4.089974	-1.410440
H	-1.702433	-4.703643	-2.372174
H	-1.097764	-5.635988	-0.973111
C	-3.633763	-4.550633	-0.401641
H	-4.371806	-3.967814	0.182079
H	-3.543950	-5.552937	0.067331
H	-4.039813	-4.687653	-1.425098
C	-2.501720	1.540213	-1.794443
C	-2.224998	1.183638	-3.143406
C	-2.090827	2.209321	-4.097789
H	-1.892947	1.952109	-5.148798
C	-2.184255	3.557462	-3.729073
H	-2.053512	4.344251	-4.488040
C	-2.434340	3.900280	-2.396440
H	-2.506945	4.961674	-2.113332
C	-2.626304	2.905382	-1.417866
C	-2.164514	-0.281897	-3.570400
H	-1.873153	-0.866843	-2.672268
C	-3.551739	-0.778900	-4.017995
H	-4.303209	-0.668365	-3.212715
H	-3.514060	-1.849894	-4.307359
H	-3.904793	-0.199766	-4.896612
C	-1.120990	-0.552350	-4.663509
H	-0.127582	-0.143517	-4.393093
H	-1.416825	-0.103943	-5.634766
H	-1.013768	-1.643624	-4.832708
C	-3.052206	3.304049	-0.006021
H	-3.019364	2.387449	0.618143
C	-2.103560	4.322036	0.633159
H	-1.064365	3.948083	0.636416
H	-2.404983	4.534328	1.680297
H	-2.101424	5.289863	0.089589
C	-4.502739	3.819681	0.002966
H	-5.208987	3.063283	-0.391509
H	-4.601914	4.730698	-0.623326
H	-4.822389	4.081256	1.033113
C	2.018914	0.223592	0.108859
C	2.652397	1.483677	-0.106315
C	4.059915	1.586426	-0.213720
H	4.501314	2.585388	-0.349829
C	4.881830	0.457769	-0.175852
H	5.972760	0.553183	-0.289937
C	4.289062	-0.791352	0.027556
H	4.906652	-1.700441	0.089381
C	2.892656	-0.905256	0.196779
C	1.956871	2.805653	-0.249659
C	1.633229	3.567113	0.907209
C	1.216051	4.901051	0.741210
H	0.978033	5.510689	1.625208
C	1.079789	5.462916	-0.534914
H	0.731849	6.501843	-0.643079
C	1.377608	4.699952	-1.668439
H	1.268910	5.147002	-2.668520
C	1.846925	3.377334	-1.546450
C	1.816581	2.980734	2.305787
H	1.704034	1.879945	2.208422
C	0.766046	3.471851	3.311420
H	-0.263792	3.345600	2.923388
H	0.903980	4.544599	3.559584
H	0.850298	2.908607	4.263429
C	3.237171	3.255072	2.834146
H	4.009379	2.834995	2.161233
H	3.379704	2.806957	3.839856
H	3.415774	4.347491	2.919264
C	2.315223	2.622699	-2.789440
H	2.517114	1.575906	-2.482175
C	1.252158	2.574697	-3.890579
H	0.310023	2.137496	-3.515475
H	1.606439	1.965718	-4.748364
H	1.011572	3.584818	-4.282866
C	3.633958	3.209972	-3.324788
H	4.436055	3.183508	-2.561678
H	3.499942	4.267376	-3.634911
H	3.986502	2.640629	-4.209835
C	2.428326	-2.280840	0.584783
C	2.497766	-2.614046	1.972533
C	2.296131	-3.948404	2.364718
H	2.348275	-4.212115	3.431356

C	2.052280	-4.947849	1.417482
H	1.902361	-5.990116	1.738492
C	1.986788	-4.616120	0.061650
H	1.794164	-5.403171	-0.684476
C	2.168746	-3.290787	-0.384365
C	2.919823	-1.579390	3.015828
H	2.810632	-0.577099	2.553995
C	2.053843	-1.596809	4.281454
H	0.985643	-1.459786	4.037335
H	2.363158	-0.781840	4.967322
H	2.150739	-2.550606	4.840413
C	4.405934	-1.758845	3.377270
H	5.054406	-1.667828	2.485153
H	4.586064	-2.756586	3.829537
H	4.723878	-0.988764	4.110046
C	2.150590	-3.066077	-1.898203
H	1.641973	-3.966448	-2.306670
C	1.347668	-1.854905	-2.395405
H	0.374939	-1.747667	-1.859513
H	1.109648	-1.972006	-3.470569
H	1.900949	-0.904567	-2.275369
C	3.566530	-3.065482	-2.507615
H	4.139072	-3.962027	-2.195894
H	4.137161	-2.167519	-2.199117
H	3.508034	-3.064130	-3.615849

Conformation 28.
Multiplicity: 5
Charge: 0
E(B97-3c) = -3593.859555228174 Hartree
E(GFN1-xTB) = -169.710873146138 Hartree
E(GFN2-xTB) = -169.235896181251 Hartree
E(GFN-FF) = -24.044662880788 Hartree
E(M06/def2-TZVP) = -3593.609560879721 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3592.323967382504 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3592.628407848730 Hartree
E(PBEh-3c) = -3588.829809006462 Hartree
E(PM6) = 182.74979 Kcal/mol
E(PM7) = 67.32603 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3596.386623643481 Hartree

Coordinates:

Fe	0.273286	0.079639	0.045997
C	-0.500405	1.983685	0.119988
C	-1.398008	2.776463	-0.653267
C	-1.957892	3.959192	-0.112348
H	-2.662100	4.534831	-0.732843
C	-1.614336	4.422236	1.161430
H	-2.056512	5.350016	1.555391
C	-0.659524	3.716905	1.899403
H	-0.303227	4.105076	2.866508
C	-0.119259	2.518362	1.388849
C	-1.723275	2.616603	-2.114425
C	-2.908357	1.980166	-2.576690
C	-3.292360	2.159316	-3.920188
H	-4.215031	1.671561	-4.273452
C	-2.528305	2.928557	-4.805907
H	-2.854618	3.060383	-5.848836
C	-1.336765	3.507526	-4.359404
H	-0.721220	4.095181	-5.058282
C	-0.919890	3.367408	-3.020983
C	-3.751899	1.040225	-1.721128
H	-4.613855	0.758080	-2.364823
C	-4.348056	1.645402	-0.438799
H	-4.808591	2.634509	-0.633414
H	-3.587052	1.778396	0.353531
H	-5.135778	0.976045	-0.038611
C	-2.972936	-0.252130	-1.433852
H	-2.573515	-0.700966	-2.364012
H	-3.612737	-1.005259	-0.936496
H	-2.107808	-0.058430	-0.761603
C	0.360784	4.063845	-2.565945
H	0.531134	3.783747	-1.508809
C	1.585245	3.582722	-3.358514
H	1.713517	2.486695	-3.265393
H	2.508799	4.070046	-2.981788
H	1.501548	3.823290	-4.439164
C	0.215978	5.593523	-2.611002
H	-0.634814	5.932373	-1.986724
H	0.040965	5.954957	-3.645888
H	1.135368	6.086537	-2.232347
C	0.954964	1.848819	2.193034
C	2.307857	1.924036	1.729543
C	3.329393	1.415542	2.558654
H	4.375542	1.473283	2.229598
C	3.036868	0.863219	3.807452
H	3.848946	0.471391	4.438842
C	1.713144	0.816451	4.264725
H	1.506804	0.399733	5.259254
C	0.653054	1.309276	3.484731
C	2.674723	2.660757	0.435373
H	1.936291	2.354233	-0.337926
C	2.544557	4.186520	0.609668
H	1.513194	4.493823	0.862316
H	2.833149	4.703590	-0.328410
H	3.218912	4.541806	1.416543
C	4.071241	2.326964	-0.098547
H	4.240455	1.237768	-0.166365
H	4.868793	2.763656	0.538136
H	4.194909	2.748343	-1.115966
C	-0.778969	1.316695	4.027212
H	-1.130927	2.368543	3.962979
C	-1.732047	0.469568	3.170215
H	-1.783086	0.828687	2.124575
H	-2.759208	0.501649	3.585318
H	-1.406861	-0.585204	3.157990
C	-0.890455	0.897209	5.497735
H	-0.249367	1.510359	6.162572
H	-0.621202	-0.170187	5.636556
H	-1.938228	1.013977	5.839006
C	-0.004666	-1.942814	-0.141227
C	-0.734295	-2.935092	0.582295
C	-1.005732	-4.189959	-0.014561
H	-1.564487	-4.938231	0.568284
C	-0.533976	-4.517903	-1.289503
H	-0.752699	-5.504083	-1.726548
C	0.272337	-3.600613	-1.970963
H	0.726320	-3.870634	-2.935842
C	0.535317	-2.334950	-1.408713
C	-1.149459	-2.834886	2.025368
C	-2.527718	-2.831403	2.379562
C	-2.891799	-2.887292	3.739803
H	-3.957630	-2.876407	4.015129
C	-1.923345	-2.946500	4.743064
H	-2.221219	-2.983149	5.802198
C	-0.566890	-2.961751	4.393721
H	0.187826	-3.021879	5.189510
C	-0.153950	-2.919084	3.048822
C	-3.637758	-2.763255	1.335986
H	-3.154045	-2.616231	0.349578
C	-4.574235	-1.568879	1.580927
H	-4.012864	-0.615513	1.610047
H	-5.120954	-1.669558	2.541006
H	-5.335293	-1.496609	0.776698
C	-4.435679	-4.077244	1.269816
H	-3.780165	-4.943091	1.050637
H	-5.210323	-4.026484	0.476988
H	-4.950733	-4.283727	2.231072
C	1.333041	-3.032151	2.710899
H	1.528255	-2.298656	1.900227
C	2.265145	-2.693638	3.879658
H	2.018716	-1.716267	4.331898
H	3.314052	-2.644258	3.525847
H	2.225544	-3.469043	4.672754
C	1.684421	-4.432814	2.171808
H	1.130115	-4.684644	1.248836
H	1.452152	-5.206906	2.932498
H	2.768338	-4.497492	1.943613
C	1.513170	-1.431901	-2.105520
C	2.815063	-1.282656	-1.529270
C	3.756223	-0.460245	-2.179247
H	4.767669	-0.360465	-1.758324
C	3.445545	0.184679	-3.380247
H	4.189813	0.831276	-3.869884
C	2.199782	-0.032297	-3.982234
H	1.980600	0.433740	-4.954519
C	1.228781	-0.852188	-3.377852
C	3.276248	-2.195517	-0.395804
H	2.369501	-2.591733	0.096005
C	4.019728	-3.400705	-1.001716
H	3.384616	-3.929266	-1.740419
H	4.298443	-4.125567	-0.208929
H	4.948237	-3.080261	-1.518757
C	4.106980	-1.501075	0.684672
H	3.524070	-0.704147	1.185048
H	5.037044	-1.047177	0.283439
H	4.413446	-2.231422	1.460098
C	-0.049571	-1.175993	-4.140470
H	-0.752647	-1.646511	-3.422650
C	-0.726343	0.069646	-4.716528
H	-0.881315	0.836671	-3.938235
H	-1.715032	-0.184527	-5.147397
H	-0.126408	0.528610	-5.528937
C	0.236990	-2.196882	-5.258623
H	0.704905	-3.123949	-4.873236
H	0.928015	-1.766388	-6.013083
H	-0.701486	-2.476633	-5.780163

Conformation 29.
Multiplicity: 5
Charge: 0
E(B97-3c) = -3593.858900479013 Hartree

E(GFN1-xTB) = -169.706134784175 Hartree
E(GFN2-xTB) = -169.221632009004 Hartree
E(GFN-FF) = -24.131474225878 Hartree
E(M06/def2-TZVP) = -3593.604869074244 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3592.326692080129 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3592.618860379635 Hartree
E(PBEh-3c) = -3588.816441902036 Hartree
E(PM6) = 155.92226 Kcal/mol
E(PM7) = 58.16683 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3596.371327932491 Hartree

Coordinates:

Fe	0.301122	0.343081	-0.113376
C	-0.506948	0.423135	1.702542
C	-1.893170	0.569453	2.020188
C	-2.409493	-0.056559	3.176670
H	-3.484027	0.042679	3.398849
C	-1.574773	-0.760149	4.057430
H	-1.998043	-1.251649	4.946744
C	-0.191959	-0.764224	3.839494
H	0.485092	-1.215699	4.581496
C	0.350823	-0.160720	2.682982
C	-2.859539	1.504286	1.326192
C	-3.815889	1.054050	0.377667
C	-4.868161	1.910168	-0.004971
H	-5.620565	1.549625	-0.723035
C	-4.976695	3.203804	0.512514
H	-5.809460	3.856611	0.209140
C	-4.002260	3.668189	1.402353
H	-4.073987	4.692533	1.799157
C	-2.943238	2.840154	1.821432
C	-3.776849	-0.354720	-0.194196
H	-2.816857	-0.805657	0.121053
C	-3.809244	-0.353026	-1.729848
H	-2.931658	0.178153	-2.146673
H	-4.725400	0.130617	-2.125993
H	-3.787554	-1.387032	-2.123814
C	-4.910013	-1.208541	0.399821
H	-4.839478	-1.252316	1.505264
H	-4.871398	-2.245932	0.011077
H	-5.904423	-0.787408	0.143418
C	-1.967804	3.371700	2.865106
H	-1.131860	2.649932	2.926360
C	-1.370575	4.731059	2.473096
H	-0.876691	4.676392	1.483167
H	-0.614858	5.052248	3.219105
H	-2.140932	5.528397	2.428322
C	-2.627567	3.426008	4.253927
H	-2.995749	2.426680	4.559346
H	-3.491377	4.123255	4.261792
H	-1.903678	3.770431	5.021043
C	1.854884	-0.055611	2.596157
C	2.490845	1.197982	2.877655
C	3.894365	1.242068	2.968003
H	4.391404	2.196486	3.190059
C	4.674920	0.090322	2.805428
H	5.770588	0.148470	2.894738
C	4.054440	-1.126029	2.516905
H	4.667148	-2.028040	2.369364
C	2.652675	-1.216657	2.397738
C	1.681396	2.459815	3.165751
H	0.833067	2.461499	2.448665
C	1.100893	2.421261	4.592830
H	0.431243	1.554222	4.744034
H	0.519675	3.342041	4.802874
H	1.919478	2.358179	5.339566
C	2.460533	3.766697	2.967757
H	2.985935	3.803339	1.993642
H	3.218769	3.921528	3.763410
H	1.765450	4.628497	3.012202
C	2.035853	-2.560096	2.039557
H	0.966826	-2.378890	1.810782
C	2.680219	-3.144865	0.777393
H	2.615396	-2.429924	-0.065105
H	2.163400	-4.072073	0.469300
H	3.750057	-3.394441	0.933444
C	2.102663	-3.560147	3.205276
H	1.588738	-3.175379	4.107994
H	3.154840	-3.778737	3.483697
H	1.623229	-4.519351	2.919779
C	0.076856	-0.864573	-1.737048
C	-0.178139	-2.149315	-2.295685
C	-0.780968	-2.226664	-3.574130
H	-1.022446	-3.220677	-3.982268
C	-1.002371	-1.085750	-4.357273
H	-1.439733	-1.186550	-5.362204
C	-0.594195	0.170561	-3.893577
H	-0.659172	1.043346	-4.556355
C	-0.073619	0.288969	-2.587334
C	0.390076	-3.462861	-1.797686
C	-0.274717	-4.390632	-0.944841
C	0.323705	-5.644565	-0.700130
H	-0.200441	-6.352101	-0.038161
C	1.540292	-6.010901	-1.283076
H	1.979204	-7.000082	-1.082487
C	2.189899	-5.101913	-2.121151
H	3.148157	-5.380011	-2.585187
C	1.640470	-3.832932	-2.386120
C	-1.624997	-4.145082	-0.279831
H	-1.853343	-5.082896	0.271749
C	-2.759780	-3.965111	-1.299655
H	-2.764311	-4.794893	-2.034804
H	-2.661487	-3.017094	-1.859394
H	-3.743580	-3.957987	-0.788095
C	-1.564908	-3.026519	0.767892
H	-0.862379	-3.285354	1.583203
H	-2.558367	-2.851221	1.225983
H	-1.217389	-2.072423	0.326294
C	2.403629	-2.912343	-3.340746
H	1.943772	-1.906624	-3.283373
C	3.884708	-2.762111	-2.955635
H	4.003447	-2.453184	-1.898633
H	4.372759	-1.999196	-3.595730
H	4.446365	-3.708941	-3.092488
C	2.266766	-3.388979	-4.797584
H	1.205313	-3.431237	-5.109982
H	2.697952	-4.403613	-4.927941
H	2.799349	-2.701963	-5.487420
C	0.381083	1.583791	-1.961064
C	1.693472	1.584060	-1.312093
C	2.038167	2.708686	-0.511582
H	3.003752	2.704984	0.011932
C	1.199137	3.814834	-0.407710
H	1.481144	4.661399	0.235125
C	0.012893	3.866003	-1.159666
H	-0.607417	4.772207	-1.117462
C	-0.410395	2.788168	-1.949232
C	2.814649	0.639222	-1.780534
H	2.388923	-0.376960	-1.886784
C	3.273058	1.091849	-3.178638
H	2.436241	1.066235	-3.904966
H	4.077607	0.428877	-3.557514
H	3.667385	2.128955	-3.146637
C	3.990832	0.540483	-0.807604
H	3.661539	0.282304	0.216985
H	4.570230	1.484929	-0.750389
H	4.692034	-0.248281	-1.143948
C	-1.658303	2.950440	-2.805409
H	-2.069132	1.938215	-2.994532
C	-2.761716	3.774086	-2.131333
H	-2.960502	3.422611	-1.104082
H	-3.705544	3.692744	-2.706814
H	-2.504694	4.852542	-2.083535
C	-1.283345	3.580975	-4.162630
H	-0.473591	3.030353	-4.681543
H	-0.923056	4.620264	-4.015494
H	-2.164621	3.618274	-4.835683

Conformation 30.
Multiplicity: 5
Charge: 0
E(B97-3c) = -3593.859560649872 Hartree
E(GFN1-xTB) = -169.715344862263 Hartree
E(GFN2-xTB) = -169.241268869526 Hartree
E(GFN-FF) = -24.040024822118 Hartree
E(M06/def2-TZVP) = -3593.609797125480 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3592.322026355394 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3592.626453187046 Hartree
E(PBEh-3c) = -3588.822948795612 Hartree
E(PM6) = 168.20229 Kcal/mol
E(PM7) = 59.27699 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3596.382656836694 Hartree

Coordinates:

Fe	-0.318772	-0.220240	-0.159804
C	-1.410219	1.440588	-0.732775
C	-1.344691	2.859027	-0.814902
C	-2.503296	3.613610	-1.121625
H	-2.414567	4.709454	-1.189796
C	-3.754872	3.007890	-1.276690
H	-4.648789	3.618343	-1.475565
C	-3.855706	1.616662	-1.160762
H	-4.831832	1.116019	-1.252398
C	-2.696125	0.852022	-0.928917
C	-0.123193	3.672603	-0.503715
C	0.879624	3.891575	-1.487387
C	1.956276	4.742500	-1.177278
H	2.735665	4.928374	-1.930618
C	2.052953	5.359213	0.077999
H	2.907926	6.015544	0.303865
C	1.053700	5.150792	1.035559
H	1.125386	5.648554	2.015529

C	-0.053047	4.324036	0.758640
C	0.740654	3.276192	-2.877242
H	0.218666	2.306140	-2.740334
C	2.077063	2.998057	-3.576290
H	2.757310	2.391462	-2.946996
H	2.604876	3.936103	-3.845964
H	1.904963	2.447449	-4.523536
C	-0.156096	4.154689	-3.770399
H	-1.161416	4.289591	-3.327403
H	-0.285138	3.694279	-4.772103
H	0.295242	5.159167	-3.909570
C	-1.169295	4.191875	1.792952
H	-1.933040	3.512118	1.367998
C	-0.683727	3.556269	3.099540
H	-0.218069	2.570931	2.915037
H	-1.528845	3.411700	3.803972
H	0.072259	4.186886	3.609696
C	-1.862995	5.541833	2.039516
H	-2.253662	5.974142	1.096273
H	-1.166425	6.282920	2.483932
H	-2.714121	5.419634	2.740995
C	-2.795639	-0.647203	-0.883609
C	-2.882643	-1.340750	0.366167
C	-3.019325	-2.746491	0.332244
H	-3.131141	-3.283346	1.285984
C	-3.048197	-3.454914	-0.869180
H	-3.134797	-4.550479	-0.860331
C	-2.975141	-2.767440	-2.086594
H	-3.010420	-3.333590	-3.027413
C	-2.866242	-1.367795	-2.120997
C	-3.082530	-0.689083	1.741797
H	-2.890819	-1.510727	2.465481
C	-2.154218	0.461484	2.146202
H	-1.073145	0.241645	1.970044
H	-2.239734	0.648439	3.235894
H	-2.394834	1.405054	1.627103
C	-4.555725	-0.271597	1.915204
H	-5.241938	-1.115217	1.704039
H	-4.810088	0.559867	1.227961
H	-4.740152	0.075596	2.952486
C	-2.921093	-0.629908	-3.458258
H	-2.456109	0.366454	-3.303101
C	-2.167280	-1.333693	-4.594646
H	-1.128375	-1.577722	-4.312750
H	-2.139576	-0.681329	-5.490653
H	-2.663628	-2.278661	-4.897067
C	-4.384292	-0.398079	-3.885386
H	-4.951182	0.175317	-3.129713
H	-4.903239	-1.366899	-4.038906
H	-4.425072	0.164955	-4.840358
C	1.359129	-1.254044	0.428188
C	1.818175	-2.350451	-0.368311
C	3.143723	-2.829286	-0.274351
H	3.455029	-3.661742	-0.924140
C	4.037873	-2.293065	0.657634
H	5.068058	-2.673611	0.730728
C	3.578233	-1.304022	1.531161
H	4.234251	-0.924400	2.329100
C	2.268722	-0.781695	1.420453
C	0.914325	-3.196216	-1.223519
C	0.751337	-2.993605	-2.621190
C	0.042283	-3.958394	-3.365730
H	-0.072280	-3.809978	-4.451164
C	-0.501165	-5.096795	-2.760691
H	-1.045446	-5.837963	-3.366228
C	-0.341832	-5.287496	-1.384418
H	-0.756760	-6.190253	-0.909141
C	0.367840	-4.358239	-0.600415
C	1.356198	-1.817529	-3.386935
H	0.912370	-1.879332	-4.404625
C	2.879689	-1.934056	-3.577413
H	3.155482	-2.919351	-4.003456
H	3.415838	-1.811348	-2.617053
H	3.241475	-1.146041	-4.269849
C	0.976759	-0.439357	-2.829514
H	-0.112261	-0.368946	-2.612507
H	1.208617	0.357148	-3.562461
H	1.540983	-0.197442	-1.906342
C	0.646025	-4.679281	0.869116
H	1.113062	-3.783819	1.320946
C	-0.618547	-4.979769	1.683760
H	-1.292993	-4.104038	1.698574
H	-0.350313	-5.222757	2.732534
H	-1.186523	-5.843746	1.279826
C	1.664538	-5.826947	0.986122
H	2.602805	-5.586576	0.449225
H	1.262031	-6.769288	0.559611
H	1.918489	-6.015884	2.049764
C	1.921570	0.212665	2.488354
C	1.161743	-0.240624	3.612865
C	1.060350	0.591184	4.742921
H	0.487035	0.252831	5.617973
C	1.699961	1.837303	4.782740
H	1.618452	2.471514	5.678847
C	2.409582	2.284939	3.667042
H	2.878916	3.281766	3.678933
C	2.528741	1.497666	2.502087
C	0.553414	-1.645489	3.639143
H	0.206851	-1.865459	2.606334
C	1.617128	-2.699607	4.002837
H	2.458470	-2.696429	3.286098
H	1.173934	-3.716617	4.007274
H	2.026581	-2.499625	5.014672
C	-0.650433	-1.791070	4.579053
H	-1.406558	-0.997595	4.422424
H	-0.344892	-1.758059	5.645564
H	-1.141514	-2.772177	4.416470
C	3.344825	2.111299	1.359092
H	3.077775	3.189930	1.386674
C	4.859630	2.026485	1.632878
H	5.117101	2.413261	2.639182
H	5.421455	2.620336	0.882215
H	5.215868	0.978965	1.566702
C	3.033440	1.644141	-0.067559
H	1.941353	1.596509	-0.248873
H	3.470148	0.655352	-0.299506
H	3.451876	2.377666	-0.783980

Conformation 32.
Multiplicity: 5
Charge: 0
E(B97-3c) = -3593.854300309898 Hartree
E(GFN1-xTB) = -169.710364367265 Hartree
E(GFN2-xTB) = -169.235688379871 Hartree
E(GFN-FF) = -24.039690456829 Hartree
E(M06/def2-TZVP) = -3593.603649160272 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3592.318681547038 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3592.622719349496 Hartree
E(PBEh-3c) = -3588.820667468501 Hartree
E(PM6) = 187.56521 Kcal/mol
E(PM7) = 71.21472 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3596.380427035978 Hartree

Coordinates:

Fe	-0.164081	0.233145	-0.039849
C	-1.912397	-0.828594	-0.292444
C	-2.307083	-2.102350	-0.803714
C	-3.642566	-2.550115	-0.651125
H	-3.903362	-3.551007	-1.028300
C	-4.628932	-1.751245	-0.066475
H	-5.661218	-2.120637	0.030997
C	-4.284108	-0.470555	0.375150
H	-5.041839	0.192624	0.822024
C	-2.949611	-0.023425	0.273374
C	-1.487227	-3.065261	-1.627626
C	-0.652411	-4.064365	-1.052667
C	-0.161888	-5.097507	-1.876260
H	0.476605	-5.872562	-1.422759
C	-0.464802	-5.159507	-3.240531
H	-0.075293	-5.982507	-3.858972
C	-1.252590	-4.156005	-3.810238
H	-1.478147	-4.185689	-4.887596
C	-1.773699	-3.109974	-3.024905
C	-0.182711	-4.059315	0.397773
H	0.342419	-5.030160	0.533645
C	-1.286732	-4.008389	1.466494
H	-2.079007	-4.756506	1.264016
H	-1.768191	-3.014682	1.521071
H	-0.854742	-4.229497	2.463994
C	0.872481	-2.962899	0.601335
H	1.649089	-2.989762	-0.187667
H	1.370199	-3.058730	1.583243
H	0.407636	-1.950967	0.571354
C	-2.645206	-2.054844	-3.701907
H	-2.929056	-1.319894	-2.924548
C	-1.867141	-1.286918	-4.781268
H	-0.956333	-0.816800	-4.362716
H	-2.496396	-0.482435	-5.215380
H	-1.553184	-1.950277	-5.614515
C	-3.946504	-2.652860	-4.259293
H	-4.533722	-3.153117	-3.463731
H	-3.742869	-3.403312	-5.051406
H	-4.581625	-1.859613	-4.704976
C	-2.663473	1.344286	0.834564
C	-2.680431	2.506110	0.005265
C	-2.540526	3.770234	0.620221
H	-2.554293	4.669474	-0.015488
C	-2.425936	3.902590	2.005053
H	-2.330767	4.901035	2.457921
C	-2.446584	2.761897	2.818234
H	-2.370270	2.874994	3.908106
C	-2.577106	1.480472	2.259518

C	-3.032636	2.526869	-1.485132
H	-2.752323	3.549103	-1.820604
C	-2.291197	1.546870	-2.400357
H	-1.212350	1.477809	-2.150151
H	-2.355184	1.882174	-3.455313
H	-2.708727	0.527208	-2.342426
C	-4.557284	2.412929	-1.683947
H	-5.101800	3.164320	-1.078068
H	-4.919795	1.406766	-1.394277
H	-4.819446	2.572068	-2.750373
C	-2.664509	0.248087	3.154593
H	-3.422513	-0.422735	2.700129
C	-1.330801	-0.507188	3.173184
H	-1.002060	-0.796215	2.152509
H	-1.411848	-1.441452	3.764633
H	-0.540933	0.118080	3.622414
C	-3.115958	0.548115	4.589244
H	-4.057842	1.132277	4.615744
H	-2.342906	1.110229	5.153260
H	-3.286520	-0.400904	5.136018
C	1.840243	0.478776	0.370793
C	2.591570	0.449364	1.592925
C	4.000249	0.355034	1.565366
H	4.545968	0.335210	2.521009
C	4.711581	0.346828	0.359821
H	5.810214	0.280376	0.360237
C	4.007955	0.488338	-0.837380
H	4.548747	0.570871	-1.792207
C	2.595323	0.552755	-0.839090
C	2.001886	0.711312	2.951819
C	1.970123	-0.280909	3.970930
C	1.470328	0.061984	5.243760
H	1.432985	-0.703464	6.033710
C	1.003275	1.351593	5.516307
H	0.591701	1.593507	6.508409
C	1.095317	2.342602	4.530520
H	0.783927	3.371210	4.765852
C	1.627886	2.055083	3.260060
C	2.501954	-1.693018	3.747475
H	2.671863	-1.810516	2.657564
C	1.513287	-2.782235	4.194468
H	0.522348	-2.655376	3.719223
H	1.363178	-2.772952	5.293540
H	1.896273	-3.788724	3.927502
C	3.856845	-1.886843	4.453982
H	4.609597	-1.148801	4.114400
H	4.260702	-2.901617	4.258184
H	3.749243	-1.770308	5.552526
C	1.989688	3.197530	2.313608
H	2.043492	2.773699	1.293615
C	0.985357	4.350144	2.277645
H	-0.021656	3.998077	1.989750
H	1.308078	5.112710	1.539648
H	0.901585	4.868839	3.255503
C	3.399006	3.711282	2.668046
H	4.148615	2.896551	2.637768
H	3.412008	4.147714	3.688686
H	3.720651	4.496672	1.952970
C	1.939683	0.792967	-2.171422
C	2.054621	-0.181477	-3.206433
C	1.543375	0.112972	-4.484644
H	1.620344	-0.641067	-5.282546
C	0.945344	1.346299	-4.757877
H	0.549725	1.559077	-5.762837
C	0.859241	2.314034	-3.750972
H	0.405706	3.287550	-3.982431
C	1.350731	2.068504	-2.454830
C	2.755717	-1.519622	-2.993054
H	2.986468	-1.607773	-1.912291
C	1.856883	-2.701816	-3.368940
H	0.898101	-2.665234	-2.821484
H	2.349969	-3.663994	-3.125096
H	1.620930	-2.717937	-4.452750
C	4.087223	-1.580067	-3.763243
H	4.772023	-0.756195	-3.480403
H	3.918005	-1.509268	-4.857981
H	4.607860	-2.539902	-3.566473
C	1.347284	3.194606	-1.418732
H	1.074254	2.736815	-0.442918
C	2.757070	3.796208	-1.265155
H	3.501527	3.035405	-0.964271
H	2.756214	4.595473	-0.496407
H	3.090217	4.243395	-2.224734
C	0.333423	4.309818	-1.693956
H	-0.684795	3.914650	-1.866876
H	0.618647	4.921536	-2.575032
H	0.285077	4.992759	-0.823234

Conformation 6.
Multiplicity: 5
Charge: 0

E(B97-3c) = -3593.863636730184 Hartree
E(GFN1-xTB) = -169.708943157087 Hartree
E(GFN2-xTB) = -169.225720563659 Hartree
E(GFN-FF) = -24.126324792384 Hartree
E(M06/def2-TZVP) = -3593.609934844182 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3592.330664601461 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3592.624614097380 Hartree
E(PBEh-3c) = -3588.823340892234 Hartree
E(PM6) = 151.96419 Kcal/mol
E(PM7) = 55.64619 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3596.376997650897 Hartree

Coordinates:

Fe	-0.156784	0.504572	-0.386650
C	0.423675	-0.946465	-1.685348
C	1.228397	-2.098916	-1.902727
C	0.834961	-3.030941	-2.890923
H	1.427625	-3.951050	-3.014557
C	-0.257574	-2.789203	-3.736509
H	-0.521856	-3.521962	-4.514126
C	-0.976196	-1.593457	-3.629695
H	-1.761730	-1.365485	-4.360515
C	-0.645899	-0.676454	-2.607912
C	2.566034	-2.378007	-1.261117
C	2.679433	-3.052099	-0.018396
C	3.952612	-3.444186	0.441959
H	4.037372	-3.974773	1.402985
C	5.103077	-3.194597	-0.311765
H	6.088828	-3.520891	0.053930
C	4.992171	-2.515819	-1.530393
H	5.898792	-2.306457	-2.118147
C	3.741957	-2.092318	-2.018346
C	1.450943	-3.457515	0.780208
H	0.576221	-3.005625	0.274161
C	1.480591	-2.928326	2.221364
H	1.523038	-1.821537	2.241396
H	2.355101	-3.315613	2.783964
H	0.570373	-3.233133	2.774346
C	1.278182	-4.986077	0.729109
H	1.196179	-5.343120	-0.317480
H	0.365785	-5.303951	1.272469
H	2.142535	-5.504638	1.193130
C	3.683989	-1.364498	-3.358959
H	2.676884	-0.911211	-3.440346
C	4.709946	-0.224205	-3.460533
H	4.655536	0.456412	-2.588752
H	4.528267	0.374621	-4.376695
H	5.749311	-0.607776	-3.522819
C	3.843119	-2.341665	-4.537261
H	3.056127	-3.120027	-4.525915
H	4.827294	-2.853371	-4.496255
H	3.778711	-1.804144	-5.506100
C	-1.339220	0.633749	-2.349913
C	-0.492695	1.806592	-2.157062
C	-1.087573	2.948557	-1.546445
H	-0.444376	3.823746	-1.365762
C	-2.445490	3.001116	-1.248570
H	-2.867819	3.894247	-0.765949
C	-3.283652	1.940617	-1.641138
H	-4.367361	2.029146	-1.483775
C	-2.769462	0.771015	-2.215902
C	0.857102	2.068316	-2.865683
H	0.793477	3.149465	-3.120444
C	2.077108	1.923098	-1.946860
H	1.943133	2.496998	-1.008901
H	2.994643	2.305511	-2.438371
H	2.250053	0.859509	-1.683984
C	1.030284	1.336415	-4.200548
H	0.146173	1.472512	-4.855074
H	1.185524	0.250092	-4.069817
H	1.917151	1.740652	-4.729953
C	-3.721948	-0.281809	-2.764588
H	-3.228719	-1.270396	-2.657345
C	-5.070749	-0.356946	-2.042854
H	-4.946370	-0.463539	-0.951139
H	-5.646934	-1.230711	-2.408820
H	-5.692902	0.541147	-2.237018
C	-3.956866	-0.012728	-4.267733
H	-3.012718	0.104818	-4.835192
H	-4.529379	0.928833	-4.397762
H	-4.541975	-0.834683	-4.729364
C	-0.438306	0.589948	1.597255
C	-1.411868	-0.169940	2.318846
C	-1.166040	-0.536480	3.660844
H	-1.912913	-1.150583	4.188910
C	-0.015448	-0.102483	4.333026
H	0.166307	-0.405193	5.375456
C	0.858009	0.781611	3.690131
H	1.703614	1.220538	4.241252
C	0.648905	1.145417	2.340898
C	-2.800362	-0.488744	1.816426

C	-3.137356	-1.759607	1.281793
C	-4.490814	-2.079456	1.056409
H	-4.750356	-3.071959	0.656978
C	-5.507245	-1.163637	1.343239
H	-6.560856	-1.431169	1.169626
C	-5.173281	0.102172	1.838253
H	-5.973403	0.824681	2.059102
C	-3.833964	0.458392	2.084801
C	-2.079019	-2.825174	1.046488
H	-1.095213	-2.329879	1.171154
C	-2.130624	-3.412534	-0.371545
H	-1.941055	-2.633692	-1.135448
H	-3.112909	-3.879612	-0.590045
H	-1.359004	-4.197685	-0.500130
C	-2.197927	-3.921018	2.120475
H	-2.103180	-3.495633	3.139488
H	-1.410696	-4.691063	1.995661
H	-3.181517	-4.431267	2.059519
C	-3.532675	1.807084	2.730320
H	-2.452748	2.000171	2.585549
C	-4.300653	2.970405	2.087480
H	-4.137990	3.002548	0.993242
H	-3.964312	3.936955	2.515791
H	-5.393088	2.900920	2.268769
C	-3.789254	1.755023	4.247243
H	-3.177805	0.968905	4.730698
H	-4.856738	1.538827	4.461740
H	-3.532588	2.724792	4.721576
C	1.529542	2.217675	1.754869
C	2.918521	1.989856	1.544997
C	3.725317	3.039595	1.060556
H	4.798068	2.860587	0.894223
C	3.184753	4.294517	0.776856
H	3.825393	5.100532	0.387169
C	1.821843	4.527142	1.002716
H	1.411541	5.526964	0.804892
C	0.979567	3.519451	1.508473
C	3.577628	0.647678	1.837587
H	2.770255	-0.093093	2.006538
C	4.419264	0.148157	0.658042
H	3.813395	0.067434	-0.263335
H	4.824196	-0.858442	0.871087
H	5.279949	0.815980	0.448101
C	4.431271	0.713340	3.117128
H	3.839184	1.032319	3.997465
H	5.266107	1.435194	2.997735
H	4.872216	-0.279769	3.341280
C	-0.462398	3.861652	1.885444
H	-1.095677	3.024662	1.521454
C	-0.615513	3.942940	3.417683
H	-0.353082	2.989669	3.912214
H	-1.661200	4.191435	3.691602
H	0.041992	4.736949	3.828487
C	-0.998077	5.158085	1.264551
H	-0.854375	5.203361	0.167614
H	-0.512652	6.055217	1.702029
H	-2.084122	5.247903	1.466459

Conformation 9.
Multiplicity: 5
Charge: 0
E(B97-3c) = -3593.865199182437 Hartree
E(GFN1-xTB) = -169.710101482010 Hartree
E(GFN2-xTB) = -169.224817520193 Hartree
E(GFN-FF) = -24.132752866128 Hartree
E(M06/def2-TZVP) = -3593.612487956287 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3592.333150682348 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3592.626205992720 Hartree
E(PBEh-3c) = -3588.824782696111 Hartree
E(PM6) = 152.41249 Kcal/mol
E(PM7) = 53.08478 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3596.378915123636 Hartree

Coordinates:

Fe	0.577094	-0.169639	0.162694
C	0.666207	0.170487	-1.829836
C	-0.018708	0.348229	-3.061099
C	0.574513	1.157036	-4.057097
H	0.013029	1.354796	-4.983969
C	1.888420	1.633338	-3.925771
H	2.341913	2.219452	-4.739610
C	2.650667	1.289666	-2.802544
H	3.718442	1.548938	-2.768714
C	2.038590	0.586743	-1.742113
C	-1.217469	-0.457327	-3.493004
C	-0.959900	-1.557111	-4.368584
C	-2.047126	-2.259375	-4.921521
H	-1.855150	-3.099149	-5.606852
C	-3.367258	-1.924486	-4.598060
H	-4.205457	-2.489484	-5.033811
C	-3.611741	-0.874408	-3.707462
H	-4.649537	-0.611819	-3.449664
C	-2.553702	-0.123866	-3.155136
C	0.458904	-1.994857	-4.738190
H	1.162123	-1.453509	-4.074360
C	0.803436	-1.608103	-6.186963
H	0.712772	-0.516120	-6.346104
H	0.123000	-2.110993	-6.905407
H	1.842474	-1.905746	-6.438334
C	0.686188	-3.498487	-4.509256
H	0.445291	-3.793386	-3.469022
H	1.745820	-3.762447	-4.704690
H	0.063707	-4.120125	-5.185234
C	-2.879478	1.089848	-2.299038
H	-1.913820	1.488282	-1.930737
C	-3.541561	2.175579	-3.166315
H	-2.895982	2.460206	-4.021677
H	-3.749128	3.087427	-2.571068
H	-4.507640	1.820230	-3.580829
C	-3.743941	0.750917	-1.075185
H	-3.228878	0.043727	-0.397729
H	-4.714785	0.299674	-1.367032
H	-3.966809	1.663119	-0.486386
C	2.718224	0.167062	-0.462969
C	2.539765	-1.228427	-0.062598
C	2.978317	-1.605791	1.238570
H	2.806201	-2.636698	1.575995
C	3.648713	-0.711510	2.066192
H	3.968729	-1.023345	3.071040
C	3.958775	0.579314	1.601299
H	4.551197	1.243989	2.243579
C	3.518460	1.044776	0.355720
C	2.285158	-2.337097	-1.106416
H	1.418475	-2.044045	-1.731947
C	3.508767	-2.422755	-2.036720
H	3.679600	-1.467521	-2.570921
H	3.360790	-3.217393	-2.796192
H	4.425207	-2.663242	-1.458525
C	1.961576	-3.701110	-0.493809
H	1.133673	-3.644819	0.237651
H	2.840533	-4.148080	0.015125
H	1.654582	-4.406711	-1.291166
C	3.854952	2.468395	-0.081377
H	4.195996	2.418195	-1.134256
C	2.605699	3.356806	-0.029580
H	1.784913	2.952872	-0.648384
H	2.828337	4.380489	-0.392458
H	2.239249	3.433877	1.010567
C	4.995713	3.115941	0.713780
H	5.910429	2.489681	0.726258
H	4.700246	3.319477	1.763785
H	5.256657	4.091750	0.257987
C	-0.789921	0.199170	1.564624
C	-1.293616	1.486772	1.932946
C	-2.597009	1.606440	2.463219
H	-2.973630	2.607465	2.727625
C	-3.393166	0.475947	2.693232
H	-4.409891	0.586909	3.099924
C	-2.856889	-0.797311	2.468767
H	-3.429227	-1.696889	2.743279
C	-1.559890	-0.946227	1.926568
C	-0.463034	2.746327	1.968213
C	-0.645218	3.797663	1.030158
C	0.002833	5.031287	1.239061
H	-0.144392	5.846662	0.514173
C	0.829093	5.237764	2.346793
H	1.326639	6.208287	2.496271
C	1.023535	4.196528	3.261701
H	1.665998	4.360030	4.140240
C	0.385254	2.952159	3.097743
C	-1.560324	3.649405	-0.177495
H	-1.901255	2.595846	-0.194658
C	-0.825818	3.928361	-1.499969
H	-0.015068	3.194245	-1.674977
H	-0.375267	4.941777	-1.513206
H	-1.520853	3.865096	-2.359072
C	-2.805635	4.539620	-0.023316
H	-3.359661	4.299899	0.906406
H	-3.500318	4.406811	-0.877750
H	-2.529276	5.613545	0.019603
C	0.513452	1.907086	4.200253
H	0.152692	0.948636	3.781870
C	1.958887	1.686507	4.664618
H	2.612643	1.415507	3.813069
H	2.002219	0.862966	5.406540
H	2.385347	2.585933	5.155358
C	-0.407204	2.270828	5.379139
H	-1.462422	2.351335	5.050894
H	-0.113705	3.244307	5.824341
H	-0.354864	1.499434	6.174820
C	-1.021617	-2.355219	1.869839
C	-1.523295	-3.273517	0.906582

C	-1.215755	-4.643287	1.031407
H	-1.618861	-5.355562	0.296644
C	-0.390005	-5.104548	2.058383
H	-0.156072	-6.176823	2.144051
C	0.160848	-4.190764	2.965752
H	0.827464	-4.560455	3.757156
C	-0.143285	-2.817829	2.900878
C	-2.359823	-2.808336	-0.278011
H	-2.216163	-1.711071	-0.365878
C	-1.864974	-3.430120	-1.588714
H	-0.787606	-3.227466	-1.740624
H	-2.414510	-3.006628	-2.447472
H	-2.011610	-4.529612	-1.611985
C	-3.862822	-3.068168	-0.086535
H	-4.260530	-2.542354	0.802599
H	-4.065675	-4.152581	0.037545
H	-4.426430	-2.713275	-0.973671
C	0.415101	-1.871885	3.961971
H	0.655407	-0.920214	3.442288
C	-0.634330	-1.563780	5.047553
H	-1.526623	-1.059851	4.632072
H	-0.203860	-0.902635	5.827339
H	-0.965345	-2.500795	5.541642
C	1.703765	-2.376347	4.625466
H	2.456764	-2.705249	3.883463
H	1.509462	-3.229354	5.308264
H	2.155893	-1.569736	5.236466

ONEHAS

Conformation 12.
Multiplicity: 3
Charge: 0
E(B97-3c) = -3245.807407571001 Hartree
E(M06/def2-TZVP) = -3245.833553992144 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3244.546696525168 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3244.794277672185 Hartree
E(PBEh-3c) = -3241.122784359298 Hartree
E(PM6) = -144.03455 Kcal/mol
E(PM7) = -168.29481 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3246.878545832495 Hartree
E(GFN1-xTB) = -165.443257451535 Hartree
E(GFN2-xTB) = -162.842394260921 Hartree
E(GFN-FF) = -22.329415705169 Hartree

Coordinates:

V	-0.120290	0.464668	-0.061726
O	0.294920	-2.666341	0.201537
O	-1.899268	-3.336947	0.535816
N	0.762403	0.846123	1.666870
N	-1.286121	2.079985	0.028479
N	0.984390	0.337146	-1.714138
N	-1.406749	-0.905059	0.212079
H	-2.409831	-0.696484	0.165737
C	0.847573	2.108425	2.171137
C	0.075944	3.186209	1.701326
H	0.265409	4.154179	2.184760
C	-0.997257	3.165850	0.776787
C	1.824741	2.381028	3.291854
H	1.650289	1.715012	4.159952
H	1.760760	3.431307	3.628477
H	2.860844	2.178600	2.950770
C	-1.804220	4.441130	0.659345
H	-2.619531	4.360213	-0.080383
H	-1.140416	5.278841	0.362864
H	-2.239826	4.715153	1.640872
C	1.263348	-0.218053	2.503114
C	2.593520	-0.697240	2.376504
C	3.076121	-1.605823	3.339112
H	4.112384	-1.968038	3.256871
C	2.272577	-2.047958	4.393592
H	2.675008	-2.742833	5.146283
C	0.940899	-1.623439	4.465728
H	0.296764	-2.000544	5.274310
C	0.406612	-0.724139	3.525564
C	3.501155	-0.297256	1.223970
H	2.987336	0.499120	0.651887
C	4.852332	0.267999	1.688300
H	4.722071	1.131710	2.371545
H	5.437224	0.614870	0.812768
H	5.461528	-0.492061	2.220143
C	3.689919	-1.506746	0.289512
H	4.108545	-2.371921	0.845641
H	4.390662	-1.263364	-0.532118
H	2.721714	-1.817620	-0.149530
C	-1.054632	-0.303039	3.633694
H	-1.327446	0.142556	2.657229
C	-1.272837	0.765429	4.719448
H	-0.995814	0.378815	5.722679
H	-2.340139	1.068980	4.756281
H	-0.674043	1.677329	4.528708
C	-1.980425	-1.509550	3.853700
H	-1.895119	-2.242817	3.027201
H	-3.036654	-1.180101	3.896484
H	-1.768522	-2.033953	4.808100
C	-2.508342	2.015167	-0.728295
C	-2.496344	2.235409	-2.139242
C	-3.714622	2.136045	-2.837522
H	-3.721268	2.302062	-3.923466
C	-4.914059	1.832829	-2.185142
H	-5.852737	1.765152	-2.755657
C	-4.910332	1.609958	-0.805874
H	-5.854611	1.367539	-0.294904
C	-3.723391	1.688016	-0.052964
C	-1.222102	2.606806	-2.891444
H	-0.392404	2.063721	-2.397892
C	-0.913225	4.111510	-2.789714
H	0.026531	4.345931	-3.330015
H	-0.784549	4.444706	-1.743688
H	-1.729654	4.714665	-3.239692
C	-1.237152	2.171680	-4.362943
H	-1.492112	1.099491	-4.473674
H	-0.234761	2.319483	-4.809140
H	-1.953651	2.769387	-4.965244
C	-3.799689	1.450195	1.454434
H	-2.762348	1.389955	1.839645
C	-4.509594	0.130685	1.803737
H	-5.556448	0.121566	1.439067
H	-4.546611	-0.002846	2.903286
H	-3.994835	-0.754014	1.380457
C	-4.503329	2.617443	2.172812
H	-4.029096	3.590825	1.949893
H	-4.480237	2.468893	3.272242
H	-5.567253	2.688130	1.864553
C	0.685078	-0.349302	-2.903933
C	1.328920	-0.071296	-4.138315
H	2.102130	0.707132	-4.185382
C	0.971302	-0.745537	-5.312318
H	1.496290	-0.493541	-6.248399
C	-0.049503	-1.714964	-5.336228
C	-0.710610	-1.967737	-4.115404
H	-1.534825	-2.699663	-4.087772
C	-0.356489	-1.312637	-2.933312
H	-0.912143	-1.512962	-2.008761
C	-0.413562	-2.458582	-6.596059
H	-0.025400	-1.946412	-7.498692
H	-1.512576	-2.560952	-6.708411
H	0.005194	-3.488890	-6.597809
C	2.127884	1.157053	-1.632775
C	2.026449	2.427028	-1.015805
H	1.036634	2.812922	-0.735170
C	3.164242	3.206607	-0.759095
H	3.041091	4.176166	-0.250247
C	4.444823	2.786430	-1.158639
C	4.537031	1.546069	-1.832968
H	5.524760	1.189511	-2.168617
C	3.417265	0.743219	-2.059499
H	3.530633	-0.233317	-2.549292
C	5.677590	3.603751	-0.867862
H	6.291280	3.133155	-0.068838
H	5.419027	4.625385	-0.527353
H	6.330164	3.694889	-1.760387
C	0.353765	-4.087379	0.496224
C	-1.143805	-4.544462	0.242732
C	0.784696	-4.235321	1.957192
H	1.744065	-3.704684	2.105329
H	0.920964	-5.297163	2.241487
H	0.048062	-3.773831	2.642451
C	1.379049	-4.733122	-0.432531
H	1.188751	-4.469110	-1.488970
H	1.365200	-5.836745	-0.328729
H	2.394504	-4.376959	-0.170609
C	-1.415643	-4.899219	-1.224871
H	-2.509543	-4.987933	-1.373657
H	-0.944447	-5.860222	-1.509136
H	-1.037655	-4.109946	-1.904019
C	-1.632578	-5.660682	1.160235
H	-1.586292	-5.360756	2.223080
H	-1.024321	-6.577193	1.022991
H	-2.685420	-5.907920	0.919877
B	-1.031662	-2.270614	0.335518

Conformation 14.
Multiplicity: 3
Charge: 0
E(B97-3c) = -3245.807559768978 Hartree
E(M06/def2-TZVP) = -3245.832323544536 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3244.546918780320 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3244.794067184479 Hartree
E(PBEh-3c) = -3241.121740502013 Hartree
E(PM6) = -149.80649 Kcal/mol

E(PM7) = -168.80914 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3246.878271518955 Hartree
E(GFN1-xTB) = -165.444559293266 Hartree
E(GFN2-xTB) = -162.840417247739 Hartree
E(GFN-FF) = -22.328108762868 Hartree

Coordinates:

V	-0.143516	0.063693	-0.495559
O	1.270747	-2.881901	2.293573
O	1.029832	-0.600079	2.607399
N	-1.882254	0.610287	0.236333
N	-0.963366	-0.765383	-2.117671
N	1.157776	1.526591	-0.796353
N	0.474086	-1.504231	0.379142
H	0.586779	-2.338918	-0.208641
C	-2.967546	0.854256	-0.550486
C	-3.083770	0.382172	-1.868678
H	-4.010980	0.648243	-2.394089
C	-2.200281	-0.471740	-2.573781
C	-4.089515	1.700116	0.004800
H	-4.462395	1.316497	0.974472
H	-4.933069	1.761209	-0.706279
H	-3.715787	2.727923	0.198118
C	-2.707467	-1.024984	-3.888150
H	-1.948798	-1.628477	-4.416116
H	-3.024140	-0.194732	-4.551381
H	-3.605369	-1.653000	-3.719918
C	-2.077164	0.690890	1.660803
C	-2.720745	-0.408789	2.302324
C	-3.068225	-0.282108	3.658297
H	-3.587370	-1.112927	4.160258
C	-2.759984	0.876803	4.382574
H	-3.048606	0.960531	5.441454
C	-2.057717	1.913206	3.758989
H	-1.785637	2.810755	4.335684
C	-1.700419	1.842514	2.398240
C	-3.050735	-1.692407	1.546439
H	-2.480436	-1.657258	0.597190
C	-2.587769	-2.945202	2.306614
H	-1.492072	-2.940793	2.467993
H	-2.836053	-3.857035	1.727457
H	-3.086266	-3.041791	3.293006
C	-4.544871	-1.789376	1.191218
H	-5.173041	-1.818330	2.106273
H	-4.745946	-2.715484	0.613336
H	-4.879397	-0.932665	0.574914
C	-0.911047	2.977002	1.768271
H	-0.819017	2.752789	0.689134
C	0.508390	3.018729	2.359534
H	0.481497	3.266349	3.441903
H	1.120244	3.789061	1.849961
H	1.012928	2.039307	2.249786
C	-1.613571	4.337945	1.886947
H	-2.638438	4.304616	1.464555
H	-1.043382	5.108317	1.329530
H	-1.695927	4.671912	2.942514
C	-0.160709	-1.755856	-2.784115
C	0.865545	-1.350134	-3.691197
C	1.621730	-2.353095	-4.326468
H	2.411565	-2.061420	-5.031820
C	1.393402	-3.712112	-4.083053
H	1.997026	-4.474651	-4.598113
C	0.405276	-4.093170	-3.172158
H	0.235840	-5.161653	-2.970772
C	-0.382087	-3.137962	-2.501196
C	1.140300	0.121656	-3.994593
H	1.031265	0.668086	-3.034626
C	0.122463	0.718363	-4.984164
H	0.360285	1.783792	-5.178473
H	-0.911430	0.681044	-4.598358
H	0.147225	0.175689	-5.952404
C	2.563862	0.380021	-4.504935
H	3.331066	-0.033554	-3.821970
H	2.738458	1.470823	-4.585961
H	2.725783	-0.045054	-5.517810
C	-1.449150	-3.625793	-1.521920
H	-1.809674	-2.743369	-0.956269
C	-0.893400	-4.639453	-0.504863
H	-0.543098	-5.567199	-1.001413
H	-1.686626	-4.933215	0.210301
H	-0.052094	-4.233342	0.089715
C	-2.654463	-4.241677	-2.256845
H	-3.092232	-3.546618	-2.996624
H	-3.449750	-4.517837	-1.533914
H	-2.358048	-5.163128	-2.800315
C	0.633391	2.745777	-1.261235
C	1.200809	4.003641	-0.931911
H	2.142573	4.037569	-0.366287
C	0.563866	5.194598	-1.297548
H	1.027262	6.154097	-1.015033
C	-0.661981	5.204914	-1.997115
C	-1.209572	3.954317	-2.346868
H	-2.153514	3.909950	-2.914423
C	-0.569783	2.756078	-2.011339
H	-1.011673	1.805831	-2.341700
C	-1.351432	6.492679	-2.371714
H	-0.821892	7.372733	-1.957323
H	-2.395808	6.520002	-1.995678
H	-1.405605	6.623976	-3.473690
C	2.559140	1.395906	-0.665890
C	3.442253	1.946417	-1.627775
H	3.026190	2.510843	-2.473924
C	4.826134	1.775713	-1.518869
H	5.480862	2.208901	-2.292783
C	5.399867	1.050351	-0.453821
C	4.517260	0.511735	0.503694
H	4.929877	-0.049782	1.358462
C	3.130628	0.685183	0.413408
H	2.474262	0.280407	1.194812
C	6.894007	0.893167	-0.325584
H	7.342581	1.730790	0.252611
H	7.390363	0.883740	-1.316710
H	7.162852	-0.044192	0.201177
C	1.988394	-2.570088	3.515753
C	1.426180	-1.134541	3.897406
C	3.481255	-2.554943	3.162215
H	3.751568	-3.531689	2.715976
H	4.117538	-2.387262	4.052977
H	3.705392	-1.770089	2.413500
C	1.699046	-3.658955	4.544915
H	0.612531	-3.790649	4.699702
H	2.169471	-3.416556	5.518836
H	2.113748	-4.624153	4.193457
C	0.177275	-1.189835	4.779739
H	-0.269954	-0.179308	4.828645
H	0.418989	-1.521797	5.808419
H	-0.588614	-1.867331	4.357162
C	2.456783	-0.186447	4.508218
H	3.300944	-0.000628	3.819129
H	2.856245	-0.593650	5.458696
H	1.976630	0.788128	4.726025
B	0.895139	-1.668834	1.724686

Conformation 17.
Multiplicity: 3
Charge: 0
E(B97-3c) = -3245.801539281352 Hartree
E(M06/def2-TZVP) = -3245.829049263117 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3244.540307955796 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3244.787944505697 Hartree
E(PBEh-3c) = -3241.116237118545 Hartree
E(PM6) = -148.93650 Kcal/mol
E(PM7) = -167.99316 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3246.872093387058 Hartree
E(GFN1-xTB) = -165.438439133982 Hartree
E(GFN2-xTB) = -162.835264001613 Hartree
E(GFN-FF) = -22.322441839424 Hartree

Coordinates:

V	0.127637	0.418946	0.105026
O	-2.083691	-2.896228	1.787176
O	-0.399281	-3.075856	0.205300
N	2.101772	0.254494	-0.239374
N	0.367103	1.743630	1.583545
N	-0.829279	1.099925	-1.451740
N	-0.916974	-0.820014	1.112620
H	-1.500420	-0.372342	1.833367
C	3.025810	1.121182	0.223751
C	2.721714	2.163901	1.127033
H	3.564436	2.817458	1.390029
C	1.510282	2.439037	1.796011
C	4.478498	0.995150	-0.180437
H	4.640948	0.198101	-0.926642
H	5.098349	0.771097	0.711811
H	4.848360	1.954252	-0.593966
C	1.498636	3.607116	2.757513
H	0.976646	3.367038	3.702771
H	0.944724	4.455919	2.304025
H	2.524641	3.946901	2.986820
C	2.444764	-0.793270	-1.166622
C	2.358642	-0.525978	-2.572455
C	2.539423	-1.586228	-3.478252
H	2.462165	-1.384374	-4.556611
C	2.799843	-2.886358	-3.033485
H	2.910325	-3.710838	-3.754025
C	2.937060	-3.121715	-1.664456
H	3.174567	-4.137211	-1.308055
C	2.793622	-2.096978	-0.704803
C	2.129993	0.876465	-3.124611
H	1.720457	1.493846	-2.304296
C	3.458009	1.518286	-3.571972
H	4.203567	1.556987	-2.757007

H	3.280915	2.555658	-3.922807
H	3.908662	0.946902	-4.410492
C	1.123939	0.924804	-4.284227
H	1.537105	0.463401	-5.205308
H	0.876735	1.978008	-4.522123
H	0.178291	0.407826	-4.036914
C	3.153282	-2.510726	0.725630
H	2.819778	-3.568186	0.792705
C	2.487097	-1.787998	1.895320
H	2.879621	-0.764459	2.049754
H	2.677538	-2.355523	2.829633
H	1.393200	-1.721451	1.757035
C	4.686453	-2.533844	0.897916
H	5.178979	-3.130848	0.104849
H	4.957267	-2.973389	1.880188
H	5.112852	-1.511910	0.860916
C	-0.700503	1.899541	2.545004
C	-1.761977	2.817702	2.326571
C	-2.759787	2.945025	3.312850
H	-3.580613	3.660589	3.150195
C	-2.728395	2.183744	4.484441
H	-3.517402	2.298471	5.243156
C	-1.690883	1.264069	4.680042
H	-1.672993	0.653247	5.595071
C	-0.667834	1.098753	3.729131
C	-1.860809	3.650073	1.060316
H	-0.989438	3.394858	0.430265
C	-1.802985	5.161699	1.330637
H	-1.781417	5.717900	0.371121
H	-0.899188	5.443823	1.907586
H	-2.686533	5.511002	1.904902
C	-3.120147	3.283760	0.260059
H	-3.165512	2.191480	0.087825
H	-3.113519	3.788819	-0.726897
H	-4.045112	3.583486	0.795851
C	0.446553	0.090517	3.982392
H	0.919887	-0.094980	3.002175
C	-0.075686	-1.258551	4.501789
H	-0.477820	-1.181165	5.533415
H	0.753011	-1.995189	4.532787
H	-0.871147	-1.672846	3.852125
C	1.527625	0.647713	4.925954
H	2.001235	1.562741	4.522123
H	2.329795	-0.103624	5.078904
H	1.100462	0.896116	5.920324
C	-1.683072	0.086034	-1.962544
C	-3.092230	0.226365	-2.033431
H	-3.556388	1.171510	-1.720820
C	-3.893339	-0.830205	-2.473484
H	-4.986269	-0.693523	-2.511672
C	-3.338304	-2.073519	-2.854917
C	-1.942205	-2.211770	-2.769305
H	-1.468713	-3.164867	-3.051640
C	-1.126083	-1.156130	-2.338100
H	-0.036955	-1.299294	-2.292652
C	-4.219628	-3.201916	-3.327586
H	-4.721149	-2.953240	-4.286969
H	-5.022628	-3.421866	-2.593306
H	-3.639790	-4.132552	-3.483486
C	-0.771689	2.374250	-2.019842
C	-1.586466	2.799336	-3.100102
H	-2.312891	2.102850	-3.539268
C	-1.462085	4.088479	-3.633494
H	-2.115004	4.377532	-4.473366
C	-0.527837	5.019617	-3.137500
C	0.307722	4.583556	-2.087337
H	1.075851	5.264231	-1.685425
C	0.199872	3.299463	-1.546731
H	0.895675	2.996803	-0.749074
C	-0.432490	6.418974	-3.690509
H	-1.055764	7.132310	-3.107220
H	-0.782205	6.468576	-4.741044
H	0.607654	6.801865	-3.658896
C	-2.174067	-4.239452	1.254450
C	-0.754076	-4.430495	0.578045
C	-3.320928	-4.244720	0.236140
H	-4.241127	-3.885060	0.736601
H	-3.515026	-5.258104	-0.167609
H	-3.102787	-3.559775	-0.606060
C	-2.474368	-5.202514	2.400134
H	-1.745552	-5.092825	3.224019
H	-2.460343	-6.253798	2.048173
H	-3.482439	-4.991326	2.807886
C	0.303591	-4.929506	1.570793
H	1.299135	-4.884273	1.088137
H	0.118972	-5.976725	1.879619
H	0.332668	-4.291336	2.476055
C	-0.749131	-5.299828	-0.676630
H	-1.431018	-4.900617	-1.448832
H	-1.049774	-6.340194	-0.439651
H	0.272742	-5.321936	-1.104823
B	-1.132993	-2.219760	1.023094

Conformation 22.
Multiplicity: 3
Charge: 0
E(B97-3c) = -3245.801048785473 Hartree
E(M06/def2-TZVP) = -3245.827186985248 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3244.540156876541 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3244.787684529594 Hartree
E(PBEh-3c) = -3241.115928865082 Hartree
E(PM6) = -146.90124 Kcal/mol
E(PM7) = -168.32908 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3246.871824045993 Hartree
E(GFN1-xTB) = -165.438495317643 Hartree
E(GFN2-xTB) = -162.836387569533 Hartree
E(GFN-FF) = -22.324061356567 Hartree

Coordinates:

V	0.278278	0.358105	0.114517
O	-0.887803	-2.586994	-1.359183
O	0.525673	-3.944014	-0.121773
N	0.151133	1.388990	-1.589309
N	2.103959	1.047927	0.570175
N	-1.143101	0.859788	1.353299
N	0.713678	-1.495733	0.194741
H	1.467253	-1.726457	0.857007
C	0.950375	2.432439	-1.899505
C	2.094899	2.771532	-1.149803
H	2.650254	3.648551	-1.511367
C	2.679396	2.101747	-0.049930
C	0.656643	3.300900	-3.103891
H	-0.189902	2.918878	-3.700403
H	1.549967	3.368447	-3.756008
H	0.416929	4.332977	-2.776742
C	4.009518	2.651721	0.423709
H	4.417413	2.096770	1.285963
H	3.888997	3.715790	0.712568
H	4.754699	2.626031	-0.396256
C	-0.948758	0.984292	-2.424892
C	-2.260187	1.496706	-2.158832
C	-3.353445	0.959168	-2.861856
H	-4.363041	1.340164	-2.647916
C	-3.178467	-0.039139	-3.825593
H	-4.046082	-0.463051	-4.353720
C	-1.886368	-0.473354	-4.129306
H	-1.739408	-1.228377	-4.918571
C	-0.747961	0.026124	-3.462830
C	-2.503823	2.667455	-1.212767
H	-1.604194	2.781540	-0.580393
C	-2.685575	3.974858	-2.010213
H	-1.832895	4.183468	-2.682049
H	-2.794064	4.833952	-1.316636
H	-3.599808	3.927068	-2.638214
C	-3.707964	2.478168	-0.278378
H	-4.667307	2.505716	-0.836377
H	-3.733185	3.296317	0.467889
H	-3.661510	1.523767	0.276207
C	0.593326	-0.452903	-4.029515
H	0.385059	-1.482849	-4.387559
C	1.798489	-0.570157	-3.093771
H	2.240747	0.413410	-2.842371
H	2.589946	-1.164744	-3.594786
H	1.538912	-1.077884	-2.147456
C	0.957615	0.370435	-5.282645
H	0.125884	0.390841	-6.014668
H	1.848866	-0.062147	-5.782597
H	1.198545	1.418388	-5.016911
C	2.868939	0.275750	1.519193
C	2.640677	0.428972	2.917216
C	3.381754	-0.361116	3.815373
H	3.212894	-0.240692	4.895423
C	4.322312	-1.292591	3.362691
H	4.889650	-1.903494	4.081154
C	4.530772	-1.444937	1.988713
H	5.266018	-2.182059	1.631049
C	3.820766	-0.678250	1.044732
C	1.646811	1.448035	3.445776
H	0.897329	1.597221	2.649638
C	2.307218	2.814393	3.697566
H	1.548533	3.548543	4.036733
H	2.775007	3.218571	2.779943
H	3.095301	2.737223	4.476105
C	0.890289	0.979003	4.695427
H	0.530857	-0.063053	4.583903
H	0.012122	1.633877	4.866624
H	1.519982	1.021647	5.608738
C	4.117808	-0.887382	-0.436783
H	3.394326	-0.275895	-1.007010
C	3.931412	-2.352279	-0.871148
H	4.655093	-3.023358	-0.363867
H	4.100445	-2.451884	-1.962804

H	2.911702	-2.719114	-0.650015
C	5.535156	-0.404446	-0.798413
H	5.705145	0.646789	-0.497904
H	5.704206	-0.481189	-1.892267
H	6.308229	-1.022499	-0.295938
C	-1.973936	-0.251861	1.663260
C	-2.031214	-0.806535	2.964104
H	-1.429333	-0.352857	3.763176
C	-2.835126	-1.918301	3.232642
H	-2.860805	-2.328678	4.255042
C	-3.609407	-2.530505	2.221984
C	-3.534910	-1.983560	0.927280
H	-4.127639	-2.429572	0.113059
C	-2.734897	-0.867175	0.645821
H	-2.695980	-0.467525	-0.377672
C	-4.449167	-3.748398	2.512879
H	-4.852192	-3.732142	3.545012
H	-3.850230	-4.680382	2.412805
H	-5.302038	-3.833979	1.810674
C	-1.343287	2.098449	1.968303
C	-0.526139	3.201157	1.594922
H	0.260340	3.068498	0.835615
C	-0.696484	4.461021	2.175303
H	-0.034115	5.283230	1.858869
C	-1.690568	4.704787	3.146258
C	-2.511054	3.615457	3.502462
H	-3.307136	3.763712	4.250594
C	-2.352958	2.345547	2.933942
H	-3.027956	1.532132	3.232121
C	-1.893783	6.075026	3.742206
H	-2.641257	6.665128	3.167229
H	-0.953681	6.662351	3.747567
H	-2.264614	6.016113	4.785328
C	-1.061061	-3.929910	-1.875730
C	-0.458921	-4.825168	-0.714158
C	-0.253863	-4.032335	-3.175422
H	-0.623454	-3.267671	-3.884860
H	-0.361143	-5.025894	-3.652595
H	0.821717	-3.840280	-2.992394
C	-2.543291	-4.156002	-2.160918
H	-3.158186	-3.986212	-1.259227
H	-2.724707	-5.186934	-2.526089
H	-2.880577	-3.444687	-2.940742
C	-1.485582	-5.147526	0.379057
H	-0.952856	-5.577197	1.249775
H	-2.244085	-5.878418	0.035569
H	-1.999528	-4.226316	0.715902
C	0.239929	-6.098684	-1.182069
H	1.093212	-5.872880	-1.847741
H	-0.465524	-6.763928	-1.719711
H	0.631178	-6.651499	-0.305393
B	0.123948	-2.640013	-0.404967

Conformation 23.
Multiplicity: 3
Charge: 0
E(B97-3c) = -3245.793225753192 Hartree
E(M06/def2-TZVP) = -3245.817524484608 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3244.533924957005 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3244.780760643286 Hartree
E(PBEh-3c) = -3241.106749211474 Hartree
E(PM6) = -142.86329 Kcal/mol
E(PM7) = -161.26403 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3246.864639838727 Hartree
E(GFN1-xTB) = -165.433160972686 Hartree
E(GFN2-xTB) = -162.827517342368 Hartree
E(GFN-FF) = -22.315109370906 Hartree

Coordinates:

V	0.327300	0.008867	-0.437446
O	-1.581615	0.880722	2.419084
O	-2.554424	2.687223	1.348706
N	2.027873	0.036468	0.561627
N	1.086611	0.871045	-2.078513
N	-0.436301	-1.795015	-0.646340
N	-0.902330	1.361129	0.070924
H	-1.166695	1.972223	-0.713379
C	3.238468	0.169524	-0.038345
C	3.396343	0.550653	-1.386775
H	4.434344	0.607588	-1.740210
C	2.415074	0.955895	-2.322358
C	4.494955	-0.149462	0.738290
H	4.385190	0.066250	1.816556
H	5.363697	0.406748	0.340758
H	4.716726	-1.234071	0.646733
C	2.906400	1.559414	-3.621290
H	2.300017	1.237289	-4.487319
H	3.964821	1.293873	-3.798414
H	2.834089	2.666893	-3.587880
C	1.923841	-0.036544	1.996939
C	2.029576	1.169575	2.753944
C	1.865564	1.105367	4.148258
H	1.947534	2.031759	4.737673
C	1.602614	-0.105750	4.798338
H	1.468151	-0.131960	5.890575
C	1.535686	-1.285002	4.050489
H	1.365019	-2.244258	4.562217
C	1.709709	-1.282725	2.652867
C	2.374345	2.510455	2.115198
H	2.450899	2.350006	1.024200
C	1.285255	3.569318	2.343510
H	0.315813	3.249209	1.916133
H	1.567631	4.526362	1.860439
H	1.138659	3.773496	3.423797
C	3.741755	3.027370	2.598881
H	3.725672	3.261241	3.683722
H	4.015785	3.958074	2.060654
H	4.547127	2.286081	2.428710
C	1.767476	-2.611403	1.913806
H	1.746336	-2.391557	0.831018
C	0.580958	-3.532976	2.225470
H	0.571589	-3.845803	3.290587
H	0.642796	-4.450685	1.608010
H	-0.386203	-3.045830	2.001984
C	3.093677	-3.340067	2.203722
H	3.971878	-2.697889	1.997743
H	3.176305	-4.248096	1.571929
H	3.154368	-3.653743	3.267038
C	0.189454	1.437976	-3.057600
C	-0.077814	2.841412	-3.096085
C	-0.897074	3.320838	-4.144953
H	-1.086245	4.404247	-4.203676
C	-1.455518	2.481674	-5.105769
H	-2.082906	2.895935	-5.909355
C	-1.207735	1.106748	-5.037424
H	-1.651241	0.442324	-5.791518
C	-0.390915	0.561337	-4.033562
C	0.411328	3.961056	-2.152645
H	0.801563	4.739465	-2.847829
C	1.525233	3.674396	-1.144671
H	1.736932	4.600372	-0.573665
H	2.474240	3.352382	-1.608483
H	1.214835	2.899279	-0.423360
C	-0.777293	4.613355	-1.407402
H	-1.614397	4.863173	-2.087229
H	-0.445736	5.551076	-0.916688
H	-1.176870	3.956040	-0.609527
C	-0.124174	-0.941576	-4.024364
H	-0.084435	-1.243094	-2.959801
C	1.225385	-1.320979	-4.662694
H	1.282408	-0.957141	-5.710407
H	1.341112	-2.423169	-4.669961
H	2.087215	-0.913351	-4.105214
C	-1.237017	-1.762801	-4.690929
H	-2.244232	-1.466384	-4.338163
H	-1.090290	-2.837845	-4.462051
H	-1.220754	-1.664297	-5.796535
C	0.308462	-2.880824	-1.125236
C	-0.159756	-4.219513	-1.102412
H	-1.168649	-4.431577	-0.723254
C	0.656595	-5.275557	-1.527979
H	0.257431	-6.302332	-1.487006
C	1.970996	-5.069069	-1.991411
C	2.436049	-3.736692	-2.012923
H	3.455925	-3.520912	-2.371168
C	1.631829	-2.671542	-1.601260
H	2.044342	-1.652616	-1.654842
C	2.839578	-6.208449	-2.461794
H	2.389809	-7.190567	-2.216448
H	3.848122	-6.173156	-1.999471
H	2.992625	-6.180505	-3.562584
C	-1.830554	-1.965264	-0.427888
C	-2.402338	-1.716140	0.836841
H	-1.765187	-1.373348	1.663783
C	-3.779748	-1.883444	1.041190
H	-4.196024	-1.704654	2.045400
C	-4.640620	-2.298401	0.007820
C	-4.061173	-2.549925	-1.254313
H	-4.701463	-2.877649	-2.089385
C	-2.689069	-2.390207	-1.469451
H	-2.259719	-2.602078	-2.456358
C	-6.124755	-2.443142	0.230069
H	-6.674074	-1.548159	-0.135425
H	-6.367293	-2.559173	1.304807
H	-6.537841	-3.317421	-0.312434
C	-2.443090	1.507980	3.405222
C	-3.380146	2.428161	2.511501
C	-1.559391	2.304543	4.369000
H	-0.788943	1.626206	4.782050
H	-2.150500	2.725097	5.205794
H	-1.037903	3.131070	3.853557
C	-3.172175	0.409940	4.176962

H	-3.733423	-0.259962	3.502299
H	-3.879402	0.844300	4.911669
H	-2.432572	-0.202060	4.730061
C	-4.635261	1.701625	2.009761
H	-5.125394	2.331247	1.241823
H	-5.362491	1.513475	2.824112
H	-4.372727	0.734954	1.537020
C	-3.760069	3.761285	3.150494
H	-2.866678	4.369548	3.381443
H	-4.334322	3.602255	4.085143
H	-4.395506	4.340142	2.451736
B	-1.648927	1.632782	1.252787

Conformation 27.
Multiplicity: 3
Charge: 0
E(B97-3c) = -3245.781403204910 Hartree
E(M06/def2-TZVP) = -3245.813225579809 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3244.521840173242 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3244.769945125457 Hartree
E(PBEh-3c) = -3241.094502843497 Hartree
E(PM6) = -146.60975 Kcal/mol
E(PM7) = -160.53152 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3246.853863091834 Hartree
E(GFN1-xTB) = -165.427016702338 Hartree
E(GFN2-xTB) = -162.819046830402 Hartree
E(GFN-FF) = -22.309054926778 Hartree

Coordinates:

V	0.552269	-0.058340	0.119855
O	-2.893716	-0.936093	-2.348666
O	-2.544982	1.253399	-1.686648
N	2.061006	1.296096	0.183168
N	1.799844	-1.500427	-0.571222
N	-0.154360	-0.272287	1.925447
N	-0.771146	-0.473674	-1.205268
H	-0.621983	-1.444838	-1.521017
C	3.372794	0.982894	0.156292
C	3.841294	-0.347423	0.075008
H	4.924979	-0.476658	0.193327
C	3.128577	-1.501389	-0.311985
C	4.427742	2.068102	0.146200
H	4.714046	2.284433	-0.904848
H	5.342723	1.731708	0.668713
H	4.078255	3.015961	0.591203
C	3.915645	-2.780732	-0.487583
H	3.904226	-3.124571	-1.540814
H	3.460128	-3.599661	0.104626
H	4.965266	-2.646982	-0.169698
C	1.640675	2.668902	0.281032
C	1.185582	3.299672	-0.920362
C	0.722335	4.624976	-0.868666
H	0.368060	5.105685	-1.791719
C	0.716850	5.340904	0.331715
H	0.360911	6.381827	0.360260
C	1.175374	4.721184	1.494506
H	1.177977	5.285863	2.440572
C	1.638834	3.385831	1.520389
C	1.230269	2.588596	-2.268139
H	1.238137	1.497481	-2.066046
C	-0.003572	2.873286	-3.131497
H	-0.932838	2.672529	-2.567111
H	0.000102	2.217715	-4.025198
H	-0.022306	3.920213	-3.500037
C	2.521162	2.932159	-3.031754
H	2.580932	4.023568	-3.224846
H	2.545370	2.408778	-4.008933
H	3.428001	2.638707	-2.469515
C	2.018737	2.908164	2.936758
H	2.487877	3.808444	3.393138
C	3.021805	1.766840	3.125388
H	2.638657	0.804575	2.748215
H	3.204889	1.631300	4.210479
H	3.998950	1.972807	2.653222
C	0.748946	2.616397	3.763590
H	0.012480	3.441043	3.699459
H	1.014187	2.465864	4.829673
H	0.259258	1.693503	3.408002
C	1.285995	-2.630688	-1.315272
C	1.418910	-2.684351	-2.739264
C	0.932301	-3.834074	-3.399028
H	1.038082	-3.884956	-4.494639
C	0.320026	-4.890434	-2.720572
H	-0.044187	-5.769269	-3.273656
C	0.169456	-4.808426	-1.334860
H	-0.322308	-5.626023	-0.785925
C	0.643106	-3.695159	-0.617943
C	1.937179	-1.593957	-3.691078
H	2.323250	-2.164279	-4.564399
C	3.083716	-0.681724	-3.245243
H	3.424470	-0.082488	-4.114175
H	3.958527	-1.246280	-2.871223
H	2.774732	0.027458	-2.457516
C	0.753815	-0.749933	-4.209495
H	-0.043520	-1.390449	-4.635975
H	1.094299	-0.044717	-4.995859
H	0.301970	-0.169951	-3.382710
C	0.425882	-3.649260	0.883946
H	0.897507	-2.721624	1.250982
C	1.097339	-4.814916	1.625409
H	0.629946	-5.790186	1.374686
H	1.011341	-4.666962	2.721257
H	2.176855	-4.889694	1.381326
C	-1.070012	-3.558669	1.221846
H	-1.540678	-2.700597	0.702812
H	-1.204079	-3.421834	2.314571
H	-1.612057	-4.480497	0.923932
C	0.372272	-0.927428	3.043158
C	1.687646	-1.457685	2.977869
H	2.275761	-1.323037	2.058688
C	2.263639	-2.121287	4.064607
H	3.284774	-2.522432	3.959973
C	1.579766	-2.272254	5.287919
C	0.291818	-1.704586	5.368920
H	-0.269376	-1.776555	6.315101
C	-0.303103	-1.046164	4.286114
H	-1.301564	-0.606328	4.409112
C	2.206976	-2.967402	6.470058
H	3.117725	-3.525965	6.177356
H	1.505618	-3.685963	6.942443
H	2.502669	-2.243730	7.260597
C	-1.453969	0.294747	1.930496
C	-1.626629	1.621078	1.472511
H	-0.746024	2.217629	1.189939
C	-2.900514	2.204840	1.407359
H	-2.992862	3.236866	1.035598
C	-4.045995	1.508351	1.826604
C	-3.874032	0.172799	2.260789
H	-4.757264	-0.411742	2.565781
C	-2.616167	-0.431495	2.298927
H	-2.521387	-1.479261	2.611714
C	-5.412468	2.145821	1.826656
H	-6.154364	1.518661	1.288809
H	-5.397917	3.143430	1.346915
H	-5.797321	2.276434	2.860557
C	-4.165698	-0.264843	-2.493608
C	-3.734784	1.256736	-2.519238
C	-5.007632	-0.615486	-1.259555
H	-5.077255	-1.717802	-1.178028
H	-6.034074	-0.203282	-1.325621
H	-4.527750	-0.234798	-0.336905
C	-4.844265	-0.766401	-3.765223
H	-4.180281	-0.670205	-4.643759
H	-5.781858	-0.208888	-3.964215
H	-5.100843	-1.838035	-3.650555
C	-3.330266	1.722583	-3.924150
H	-2.879153	2.731412	-3.863096
H	-4.206563	1.778529	-4.599120
H	-2.583054	1.038041	-4.371577
C	-4.753067	2.220041	-1.918444
H	-4.960594	1.975597	-0.862792
H	-5.704451	2.193418	-2.487187
H	-4.358720	3.254854	-1.958140
B	-2.029511	-0.041208	-1.713954

Conformation 30.
Multiplicity: 3
Charge: 0
E(B97-3c) = -3245.778887900713 Hartree
E(M06/def2-TZVP) = -3245.807028098133 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3244.519852550107 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3244.767704867240 Hartree
E(PBEh-3c) = -3241.093521830369 Hartree
E(PM6) = -136.19646 Kcal/mol
E(PM7) = -154.29838 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3246.851887497893 Hartree
E(GFN1-xTB) = -165.423198959961 Hartree
E(GFN2-xTB) = -162.816027443892 Hartree
E(GFN-FF) = -22.309429283128 Hartree

Coordinates:

V	-0.018082	-0.191725	-0.373391
O	0.667283	1.211190	2.580084
O	-0.558059	3.148733	2.253464
N	1.964531	-0.228420	-0.782217
N	-0.595333	0.265676	-2.242153
N	-0.988544	-1.786924	0.294937
N	-0.577431	1.415832	0.463457
H	-1.294948	1.971428	-0.017838
C	2.328285	-0.639132	-2.027745
C	1.475508	-0.614111	-3.151840
H	1.941761	-0.949427	-4.088760

C	0.184492	-0.051594	-3.297779
C	3.731648	-1.146218	-2.293224
H	4.425064	-0.937589	-1.461238
H	4.143388	-0.706404	-3.222212
H	3.691833	-2.245073	-2.440129
C	-0.275261	0.195278	-4.719492
H	-1.348123	0.445563	-4.786522
H	-0.071333	-0.695078	-5.346141
H	0.303214	1.033015	-5.160286
C	3.022095	0.118887	0.150176
C	3.673882	1.391276	0.013074
C	4.735698	1.705240	0.887669
H	5.230598	2.682384	0.770964
C	5.171679	0.831023	1.881615
H	6.004686	1.103813	2.546667
C	4.535049	-0.403072	2.002402
H	4.873113	-1.117463	2.769451
C	3.477751	-0.795015	1.154559
C	3.318801	2.553669	-0.927658
H	4.251236	3.157655	-0.950841
C	2.992882	2.275712	-2.398102
H	3.745532	1.617916	-2.873366
H	2.995672	3.237538	-2.951263
H	2.000036	1.818014	-2.541501
C	2.248991	3.447768	-0.282204
H	1.292186	2.905892	-0.163056
H	2.067962	4.345783	-0.906616
H	2.569270	3.793538	0.719531
C	2.932925	-2.193799	1.452703
H	3.699805	-2.642182	2.120514
C	2.829909	-3.150033	0.259147
H	2.072636	-2.839392	-0.480713
H	2.532526	-4.158371	0.609766
H	3.806520	-3.245353	-0.255055
C	1.649193	-2.116885	2.289188
H	1.795218	-1.484306	3.185573
H	1.329897	-3.127990	2.612367
H	0.814055	-1.681748	1.709564
C	-1.864662	0.919267	-2.458421
C	-3.063685	0.147582	-2.556394
C	-4.272432	0.820451	-2.816744
H	-5.198958	0.236499	-2.902998
C	-4.325648	2.209279	-2.968497
H	-5.283656	2.708486	-3.178608
C	-3.154215	2.956114	-2.834644
H	-3.195480	4.050888	-2.937173
C	-1.914526	2.341600	-2.571160
C	-3.074035	-1.371154	-2.411318
H	-2.288071	-1.619277	-1.672086
C	-2.734337	-2.091260	-3.729360
H	-2.744494	-3.189547	-3.577398
H	-1.733580	-1.825963	-4.114362
H	-3.476912	-1.842383	-4.516532
C	-4.400376	-1.915001	-1.861756
H	-4.699058	-1.404217	-0.925908
H	-4.297979	-2.996628	-1.643238
H	-5.227328	-1.816803	-2.595646
C	-0.683243	3.232437	-2.443936
H	0.136168	2.605091	-2.044510
C	-0.905648	4.394956	-1.460916
H	-1.719479	5.068876	-1.797442
H	0.012025	5.009760	-1.381476
H	-1.154398	4.044821	-0.439896
C	-0.235000	3.781469	-3.810321
H	-0.032362	2.973099	-4.537932
H	0.692459	4.380227	-3.701404
H	-1.013582	4.439015	-4.250166
C	-1.942535	-1.776285	1.341268
C	-1.780202	-0.979459	2.495196
H	-0.869198	-0.379670	2.617505
C	-2.759975	-0.963238	3.498444
H	-2.599058	-0.336661	4.391370
C	-3.930409	-1.739512	3.412830
C	-4.078449	-2.551275	2.267125
H	-4.978614	-3.178466	2.159469
C	-3.112856	-2.573414	1.257881
H	-3.253786	-3.219816	0.381237
C	-4.983870	-1.713989	4.491158
H	-4.674957	-1.082547	5.347069
H	-5.196422	-2.731898	4.880542
H	-5.946731	-1.311990	4.109363
C	-0.625140	-3.033399	-0.249004
C	-0.189451	-3.130298	-1.592240
H	-0.220046	-2.245740	-2.239348
C	0.282736	-4.339557	-2.120585
H	0.620466	-4.363057	-3.169398
C	0.318558	-5.516728	-1.351741
C	-0.142126	-5.425820	-0.018417
H	-0.131002	-6.326959	0.616641
C	-0.594824	-4.223012	0.527892
H	-0.926244	-4.187231	1.575016
C	0.843217	-6.815748	-1.908964
H	1.853669	-7.049493	-1.508177
H	0.927422	-6.781281	-3.012975
H	0.188713	-7.671168	-1.643185
C	0.939681	2.038913	3.739827
C	-0.207448	3.140901	3.660271
C	2.349520	2.612625	3.577348
H	3.058882	1.778702	3.416218
H	2.666601	3.181331	4.473256
H	2.416901	3.276631	2.695835
C	0.883850	1.153566	4.984397
H	-0.064877	0.589370	5.047546
H	0.998663	1.759371	5.905440
H	1.713576	0.420174	4.952675
C	-1.474887	2.749665	4.429956
H	-2.279563	3.467268	4.177078
H	-1.320312	2.769741	5.526429
H	-1.824505	1.741032	4.137342
C	0.238050	4.545344	4.060384
H	1.054332	4.911396	3.411558
H	0.585088	4.564762	5.112841
H	-0.613876	5.247001	3.965988
B	-0.165765	1.926714	1.724347

Conformation 31.
Multiplicity: 3
Charge: 0
E(B97-3c) = -3245.787408443377 Hartree
E(M06/def2-TZVP) = -3245.814781131296 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3244.527681443584 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3244.775079788862 Hartree
E(PBEh-3c) = -3241.103085665205 Hartree
E(PM6) = -134.93475 Kcal/mol
E(PM7) = -161.13247 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3246.860116028166 Hartree
E(GFN1-xTB) = -165.430664114686 Hartree
E(GFN2-xTB) = -162.829281041310 Hartree
E(GFN-FF) = -22.315125636774 Hartree

Coordinates:

V	0.071462	-0.468708	0.213491
O	0.377560	2.491289	-0.791239
O	2.274583	2.284208	-2.107296
N	0.334851	0.095048	2.126806
N	0.657887	-2.347032	0.482424
N	-1.707564	-0.422865	-0.646674
N	1.397113	0.266668	-0.917281
H	2.058941	-0.330129	-1.422402
C	0.439896	-0.833910	3.120349
C	0.451033	-2.225936	2.896747
H	0.443728	-2.843366	3.804626
C	0.603664	-2.947931	1.688439
C	0.552321	-0.378354	4.559478
H	1.437612	0.269738	4.707328
H	0.632270	-1.244902	5.239766
H	-0.321762	0.230910	4.856156
C	0.721668	-4.448888	1.815290
H	1.113864	-4.917822	0.895267
H	-0.278480	-4.882733	2.023235
H	1.376349	-4.720234	2.665865
C	0.627622	1.460871	2.509212
C	2.003140	1.846146	2.553366
C	2.349176	3.095908	3.099905
H	3.411087	3.379331	3.156222
C	1.375282	3.977656	3.571294
H	1.660060	4.947791	4.005498
C	0.028984	3.619661	3.459542
H	-0.749911	4.320700	3.798901
C	-0.383555	2.376740	2.934823
C	3.130451	0.940776	2.063416
H	2.662055	0.113694	1.495601
C	4.073920	1.672327	1.093974
H	3.537113	2.033476	0.195759
H	4.872648	0.986523	0.748016
H	4.575685	2.538525	1.571990
C	3.928656	0.328511	3.228592
H	4.374266	1.119196	3.867593
H	4.757339	-0.298922	2.842313
H	3.299441	-0.315346	3.872708
C	-1.897923	2.175261	2.838106
H	-2.327608	3.074837	3.329647
C	-2.477106	0.975852	3.600511
H	-2.114514	0.010304	3.208577
H	-3.581270	0.966536	3.499545
H	-2.241924	1.035807	4.682537
C	-2.361392	2.220344	1.376073
H	-2.058558	3.168688	0.892038
H	-3.464646	2.122362	1.311519
H	-1.918810	1.398974	0.785032
C	1.027291	-3.061444	-0.716389
C	0.003592	-3.637316	-1.537748

C	0.351291	-4.158196	-2.796795
H	-0.440046	-4.582405	-3.432097
C	1.675121	-4.162022	-3.243974
H	1.930954	-4.565513	-4.235245
C	2.675532	-3.690894	-2.393436
H	3.728456	-3.753898	-2.712531
C	2.398159	-3.148450	-1.118459
C	-1.437873	-3.805148	-1.069827
H	-1.586781	-3.159027	-0.184860
C	-1.700510	-5.264468	-0.644241
H	-2.716734	-5.355867	-0.208818
H	-0.973274	-5.629152	0.103746
H	-1.644129	-5.945209	-1.519385
C	-2.478904	-3.401776	-2.124409
H	-2.312004	-2.378096	-2.504250
H	-3.493129	-3.433942	-1.681418
H	-2.472251	-4.095431	-2.991018
C	3.666271	-2.760278	-0.333104
H	4.374703	-3.575381	-0.600955
C	3.619015	-2.749028	1.197234
H	2.993397	-1.934410	1.602555
H	4.647068	-2.600359	1.585989
H	3.248892	-3.706032	1.608969
C	4.311513	-1.463484	-0.859910
H	4.377717	-1.455139	-1.966065
H	5.340672	-1.358205	-0.459093
H	3.742191	-0.570705	-0.542184
C	-1.811129	0.239455	-1.897663
C	-1.043529	-0.206490	-2.998765
H	-0.378716	-1.072492	-2.866648
C	-1.128322	0.430644	-4.241870
H	-0.518124	0.055293	-5.078903
C	-1.986323	1.530996	-4.448524
C	-2.746332	1.975847	-3.347220
H	-3.420596	2.838809	-3.471394
C	-2.657564	1.354405	-2.095201
H	-3.251604	1.734203	-1.253075
C	-2.051381	2.232950	-5.780890
H	-1.887590	1.530707	-6.622452
H	-1.266264	3.017597	-5.857005
H	-3.027806	2.733623	-5.933790
C	-2.853491	-0.924536	-0.020198
C	-2.725537	-1.551806	1.247834
H	-1.742066	-1.609617	1.739717
C	-3.820651	-2.126200	1.898512
H	-3.661525	-2.603561	2.879168
C	-5.112323	-2.103821	1.334147
C	-5.241111	-1.486321	0.073368
H	-6.229754	-1.461991	-0.413939
C	-4.151717	-0.913671	-0.594134
H	-4.302149	-0.477836	-1.590602
C	-6.301064	-2.685245	2.056824
H	-6.797004	-1.929321	2.705077
H	-6.007730	-3.529040	2.713348
H	-7.069455	-3.055479	1.348614
C	0.727336	3.843248	-1.190205
C	1.725310	3.596717	-2.401983
C	1.395421	4.518199	0.010262
H	0.724492	4.438391	0.886107
H	1.600789	5.589277	-0.183629
H	2.345057	4.019025	0.278500
C	-0.552051	4.585292	-1.567629
H	-1.147080	4.014289	-2.303208
H	-0.317626	5.584984	-1.985138
H	-1.175575	4.730823	-0.663376
C	1.008043	3.488237	-3.751836
H	1.728663	3.124779	-4.510531
H	0.610324	4.465717	-4.088324
H	0.174354	2.763724	-3.696656
C	2.875888	4.595285	-2.490883
H	3.499540	4.584707	-1.578216
H	2.493895	5.624129	-2.646959
H	3.524674	4.336239	-3.350592
B	1.366500	1.643533	-1.275010

Conformation 33.
Multiplicity: 3
Charge: 0
E(B97-3c) = -3245.801500718708 Hartree
E(M06/def2-TZVP) = -3245.826601295537 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3244.540771413405 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3244.788119946165 Hartree
E(PBEh-3c) = -3241.116327243312 Hartree
E(PM6) = -142.54922 Kcal/mol
E(PM7) = -168.05699 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3246.872871599081 Hartree
E(GFN1-xTB) = -165.441943619768 Hartree
E(GFN2-xTB) = -162.841266423987 Hartree
E(GFN-FF) = -22.324196416754 Hartree

Coordinates:

V	0.332629	-0.340136	0.038918
O	-1.318444	2.287809	-0.505452
O	-2.259129	1.751296	-2.556145
N	2.098685	0.603033	-0.057536
N	1.056994	-2.112095	-0.466313
N	-0.687980	-0.513994	1.719852
N	-0.759149	0.092619	-1.444920
H	-1.003850	-0.601079	-2.158097
C	3.281031	-0.079403	-0.062398
C	3.373228	-1.483010	-0.110923
H	4.389891	-1.890100	-0.030609
C	2.361578	-2.440949	-0.364598
C	4.583416	0.690944	-0.016491
H	4.685882	1.366812	-0.887782
H	5.446124	0.000933	-0.003772
H	4.629772	1.338770	0.878885
C	2.812674	-3.878361	-0.490106
H	2.044728	-4.521736	-0.954950
H	3.032417	-4.285923	0.518999
H	3.748261	-3.947317	-1.077895
C	2.186923	2.006211	-0.395375
C	2.299132	2.326148	-1.784180
C	2.567380	3.654461	-2.161125
H	2.675737	3.896413	-3.229274
C	2.697389	4.666422	-1.206994
H	2.917254	5.700077	-1.513812
C	2.518790	4.352966	0.143525
H	2.588667	5.149792	0.900973
C	2.260048	3.038853	0.587284
C	2.159619	1.269811	-2.879241
H	1.731737	0.367602	-2.402083
C	1.176126	1.714454	-3.973797
H	0.173595	1.935721	-3.559465
H	1.053093	0.911509	-4.727546
H	1.536440	2.613848	-4.514123
C	3.513545	0.873551	-3.494592
H	4.026544	1.751615	-3.940071
H	3.366779	0.124879	-4.300769
H	4.192851	0.424025	-2.745644
C	2.038066	2.875526	2.092533
H	2.252350	3.880824	2.515844
C	2.982689	1.907261	2.817891
H	2.869930	0.867774	2.463920
H	2.753550	1.902292	3.902754
H	4.042014	2.213929	2.701561
C	0.564022	2.580460	2.399813
H	-0.100565	3.355723	1.973150
H	0.396970	2.528299	3.495443
H	0.250093	1.612413	1.969419
C	0.083026	-3.067778	-0.929661
C	-0.615713	-3.910465	-0.017489
C	-1.608373	-4.770067	-0.528971
H	-2.154295	-5.422104	0.169431
C	-1.906895	-4.816427	-1.893316
H	-2.689633	-5.493338	-2.267941
C	-1.195662	-4.002228	-2.782605
H	-1.420213	-4.051316	-3.857961
C	-0.195251	-3.123091	-2.330372
C	-0.295572	-3.967473	1.470732
H	0.379598	-3.122662	1.703132
C	0.437572	-5.274005	1.833628
H	0.735716	-5.258298	2.901953
H	1.348662	-5.431195	1.226822
H	-0.220413	-6.154778	1.679020
C	-1.542263	-3.821992	2.356493
H	-2.120024	-2.911090	2.114928
H	-1.242052	-3.754391	3.420562
H	-2.220300	-4.695111	2.253597
C	0.599976	-2.297300	-3.339776
H	1.002705	-1.421768	-2.792811
C	-0.255065	-1.770743	-4.502439
H	-0.624806	-2.591311	-5.150698
H	0.347323	-1.098899	-5.145611
H	-1.135899	-1.194784	-4.153013
C	1.801481	-3.091988	-3.883693
H	2.483661	-3.413880	-3.075603
H	2.387859	-2.473847	-4.594638
H	1.460559	-4.001620	-4.420704
C	-2.054956	-0.136401	1.689812
C	-2.569634	0.908159	2.491335
H	-1.893530	1.450295	3.166018
C	-3.924912	1.257320	2.432319
H	-4.297304	2.073409	3.072644
C	-4.820757	0.597469	1.566616
C	-4.299630	-0.433976	0.757122
H	-4.970024	-0.972020	0.067847
C	-2.950300	-0.799183	0.817787
H	-2.569811	-1.613242	0.183917
C	-6.269371	1.003826	1.472963
H	-6.600074	1.555495	2.374714
H	-6.933262	0.125357	1.343597

H	-6.442097	1.668659	0.597916
C	-0.077636	-0.877305	2.923754
C	1.307465	-1.194554	2.925835
H	1.890588	-1.131788	1.993746
C	1.963200	-1.610305	4.088151
H	3.038593	-1.845707	4.033258
C	1.285246	-1.730794	5.318280
C	-0.091980	-1.427970	5.315158
H	-0.665859	-1.527518	6.251302
C	-0.764183	-1.015791	4.158587
H	-1.844134	-0.821854	4.203839
C	2.001910	-2.134572	6.581931
H	2.327915	-1.247834	7.169291
H	2.911115	-2.729931	6.364036
H	1.351060	-2.737600	7.247199
C	-1.971549	3.498529	-0.971176
C	-2.943387	2.949032	-2.099681
C	-0.884994	4.426959	-1.519721
H	-0.118975	4.590487	-0.738212
H	-1.299325	5.409964	-1.818200
H	-0.372135	3.979382	-2.392031
C	-2.683195	4.152813	0.210213
H	-3.328769	3.429683	0.740784
H	-3.298090	5.011123	-0.127439
H	-1.933892	4.532691	0.932429
C	-4.301428	2.503138	-1.546554
H	-4.840204	1.940044	-2.333706
H	-4.928068	3.364091	-1.241369
H	-4.167245	1.833607	-0.676011
C	-3.131115	3.886078	-3.289155
H	-2.172123	4.097598	-3.796549
H	-3.581199	4.846640	-2.967088
H	-3.812334	3.418804	-4.027358
B	-1.434852	1.340672	-1.515828

Conformation 34.
Multiplicity: 3
Charge: 0
E(B97-3c) = -3245.778711502396 Hartree
E(M06/def2-TZVP) = -3245.806681454457 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3244.520070438693 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3244.767505271749 Hartree
E(PBEh-3c) = -3241.092875854910 Hartree
E(PM6) = -136.36198 Kcal/mol
E(PM7) = -152.75292 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3246.851627098034 Hartree
E(GFN1-xTB) = -165.421141429348 Hartree
E(GFN2-xTB) = -162.814203654987 Hartree
E(GFN-FF) = -22.309508032722 Hartree

Coordinates:

V	-0.091688	0.118184	0.473959
O	-1.575977	-2.180524	-2.849755
O	0.241233	-0.747144	-2.815797
N	1.727055	-0.648182	0.770843
N	-0.898487	-0.530795	2.213503
N	-0.204260	2.075068	0.162540
N	-1.080398	-0.953724	-0.739662
H	-1.968041	-1.322479	-0.377191
C	2.155775	-0.862204	2.047981
C	1.315311	-0.834507	3.179482
H	1.830362	-0.977593	4.139070
C	-0.097853	-0.768926	3.275219
C	3.625107	-1.121780	2.302743
H	4.046227	-1.864052	1.599025
H	3.794038	-1.470162	3.337421
H	4.199464	-0.185949	2.149689
C	-0.665792	-0.983758	4.663552
H	-1.769101	-0.964181	4.679859
H	-0.288978	-0.196514	5.347659
H	-0.320038	-1.951845	5.075059
C	2.569476	-1.166190	-0.289991
C	2.501292	-2.576371	-0.523046
C	3.409377	-3.175070	-1.413741
H	3.371540	-4.264264	-1.564896
C	4.353729	-2.416599	-2.107311
H	5.064932	-2.897330	-2.795834
C	4.368055	-1.032636	-1.924909
H	5.092502	-0.419374	-2.483741
C	3.498939	-0.372690	-1.029048
C	1.508644	-3.484051	0.196317
H	0.751622	-2.831645	0.672974
C	0.764623	-4.413262	-0.776435
H	0.177882	-3.841718	-1.521956
H	0.058199	-5.060840	-0.221786
H	1.458651	-5.084970	-1.321661
C	2.197669	-4.306461	1.300951
H	3.010497	-4.933689	0.879354
H	1.471248	-4.982504	1.795137
H	2.639819	-3.661430	2.083987
C	3.642949	1.148872	-1.003353
H	4.567299	1.344870	-1.588713
C	3.883411	1.783358	0.371272
H	3.033534	1.644228	1.062436
H	4.030394	2.876295	0.263779
H	4.797863	1.369134	0.842323
C	2.499501	1.813884	-1.783530
H	2.394346	1.369515	-2.792216
H	2.682471	2.901943	-1.892298
H	1.533313	1.690143	-1.261652
C	-2.336188	-0.640195	2.344414
C	-3.111235	0.556407	2.512354
C	-4.511800	0.461435	2.593582
H	-5.102442	1.378427	2.719688
C	-5.167508	-0.769334	2.530154
H	-6.264406	-0.824902	2.597408
C	-4.406949	-1.928017	2.395051
H	-4.913867	-2.905554	2.360808
C	-2.996220	-1.912273	2.302287
C	-2.473145	1.934531	2.660812
H	-1.580326	1.948032	2.007437
C	-2.008466	2.200086	4.104221
H	-1.538245	3.201559	4.174615
H	-1.262608	1.463506	4.448809
H	-2.868019	2.167270	4.806429
C	-3.382892	3.084449	2.207127
H	-3.763051	2.934788	1.178128
H	-2.814536	4.034845	2.225122
H	-4.249122	3.221364	2.887590
C	-2.405689	-3.323058	2.119516
H	-3.160954	-3.973580	2.611125
C	-1.079967	-3.674718	2.798507
H	-0.222677	-3.103837	2.402116
H	-0.864985	-4.750422	2.634444
H	-1.128911	-3.515202	3.891480
C	-2.407895	-3.743307	0.638061
H	-3.382078	-3.525627	0.156590
H	-2.222190	-4.833186	0.547984
H	-1.621766	-3.222600	0.063230
C	-0.996124	2.693349	-0.835606
C	-1.123156	2.131989	-2.126320
H	-0.554796	1.228809	-2.382088
C	-1.938432	2.732567	-3.093650
H	-2.006642	2.271301	-4.093154
C	-2.648942	3.922019	-2.837611
C	-2.494650	4.495790	-1.558865
H	-3.022498	5.433228	-1.318758
C	-1.690712	3.901401	-0.580505
H	-1.587793	4.381739	0.401580
C	-3.546273	4.542350	-3.878275
H	-3.158996	4.375665	-4.903723
H	-3.655955	5.634672	-3.726647
H	-4.568220	4.104798	-3.844495
C	0.598603	2.893886	0.979488
C	1.172477	4.109618	0.519081
H	0.943312	4.460412	-0.496632
C	2.032920	4.850779	1.331831
H	2.462254	5.786243	0.936645
C	2.386052	4.426796	2.633100
C	1.822585	3.220090	3.084980
H	2.067849	2.847677	4.092743
C	0.939258	2.478403	2.289045
H	0.510524	1.555655	2.700290
C	3.309445	5.247528	3.497230
H	2.814577	6.175471	3.857392
H	4.215043	5.565335	2.939983
H	3.641112	4.681837	4.389919
C	-1.210651	-1.976065	-4.238440
C	0.246921	-1.348040	-4.136213
C	-2.243216	-1.007284	-4.828908
H	-3.253919	-1.439036	-4.693104
H	-2.079392	-0.832335	-5.910203
H	-2.222315	-0.032631	-4.303504
C	-1.271550	-3.317945	-4.963227
H	-0.645612	-4.078484	-4.461648
H	-0.930824	-3.215117	-6.012976
H	-2.315530	-3.688122	-4.975215
C	1.363636	-2.393499	-4.168416
H	2.315698	-1.909772	-3.879768
H	1.481076	-2.832897	-5.178470
H	1.179754	-3.210789	-3.446460
C	0.538070	-0.250021	-5.158991
H	-0.155582	0.604116	-5.053107
H	0.464954	-0.642577	-6.192996
H	1.568174	0.129195	-5.009313
B	-0.812117	-1.299074	-2.092722

OQOQOB

Conformation 1.
Multiplicity: 2

Charge: 0
E(B97-3c) = -6287.334539666292 Hartree
E(M06/def2-TZVP) = -6287.327396830854 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -6285.147511291824 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -6285.322362667313 Hartree
E(PBEh-3c) = -6277.924860852325 Hartree
E(PM6) = 262.06750 Kcal/mol
E(PM7) = 121.09013 Kcal/mol
E(ωB97X-V/def2-TZVP) = -6289.218225469356 Hartree
E(GFN1-xTB) = -298.847191368280 Hartree
E(GFN2-xTB) = -290.685712758847 Hartree
E(GFN-FF) = -36.545250644598 Hartree

Coordinates:

Cu	0.165046	-1.124304	-0.702265
N	1.120164	0.207456	-1.893151
N	-0.423841	0.395384	0.496491
N	-0.834468	-2.448053	0.471405
N	0.844072	-2.654649	-1.846764
C	1.831796	-0.080461	-3.038626
C	2.307309	1.145040	-3.650903
H	2.878579	1.194429	-4.584260
C	1.907869	2.174738	-2.837686
H	2.079228	3.248970	-2.962553
C	1.195360	1.576172	-1.725618
C	0.718944	2.299478	-0.616339
C	-0.007775	1.709709	0.437758
C	-0.497413	2.436137	1.593073
H	-0.282799	3.488320	1.807502
C	-1.267452	1.559096	2.313902
H	-1.813866	1.730163	3.246754
C	-1.214248	0.290433	1.620002
C	-1.889737	-0.862609	2.062245
C	-1.678017	-2.143884	1.522572
C	-2.236118	-3.357396	2.084113
H	-2.939203	-3.389739	2.923495
C	-1.668215	-4.403393	1.401580
H	-1.811471	-5.476596	1.562193
C	-0.813330	-3.824516	0.381569
C	-0.075033	-4.578640	-0.554721
C	0.670740	-4.003888	-1.604196
C	1.421123	-4.782107	-2.571752
H	1.436145	-5.876757	-2.613601
C	2.076158	-3.887011	-3.378593
H	2.745482	-4.093734	-4.219857
C	1.704501	-2.560884	-2.922080
C	2.181944	-1.367775	-3.497749
C	1.026736	3.755774	-0.501302
C	-0.016477	4.726959	-0.519152
C	0.289700	6.077712	-0.238928
H	-0.528362	6.806752	-0.214367
C	1.614138	6.460814	0.007626
H	1.834091	7.518303	0.220028
C	2.654335	5.518274	-0.025520
H	3.695206	5.821209	0.161600
C	2.352660	4.173534	-0.277033
H	3.148386	3.414689	-0.273943
N	-1.308116	4.297874	-0.850779
H	-1.401504	3.402550	-1.353357
C	-2.506096	4.893612	-0.515139
O	-2.579713	5.910953	0.183967
C	-3.753325	4.245270	-1.069130
C	-4.959649	4.940293	-0.760330
H	-4.847270	5.845384	-0.146370
C	-6.197098	4.501831	-1.184406
H	-7.115577	5.036170	-0.899050
C	-6.285625	3.358608	-2.025234
C	-7.517013	2.875589	-2.549325
H	-8.452845	3.372672	-2.250339
C	-7.516853	1.803040	-3.423981
H	-8.452173	1.405359	-3.845204
C	-6.268545	1.230228	-3.791074
H	-6.240256	0.399406	-4.519680
N	-5.105894	1.635942	-3.311455
C	-5.088097	2.656354	-2.411961
C	-3.821497	3.069296	-1.850715
O	-2.670687	2.390766	-2.091340
C	-2.613967	0.971969	-2.346598
H	-3.446379	0.445668	-1.842606
H	-1.638180	0.646680	-1.936708
H	-2.669953	0.773557	-3.431685
C	-2.935364	-0.660227	3.114037
C	-4.216189	-0.193852	2.695847
C	-5.203778	0.080364	3.663606
H	-6.198742	0.418076	3.345060
C	-4.921024	-0.098314	5.023399
H	-5.702597	0.123089	5.765946
C	-3.667046	-0.571502	5.442151
H	-3.455049	-0.719325	6.511148
C	-2.683728	-0.854724	4.482157
H	-1.690611	-1.217263	4.787711
N	-4.426615	-0.097347	1.314330
H	-3.768084	-0.645966	0.749374
C	-5.394274	0.470653	0.510656
O	-5.449589	0.127638	-0.677083
C	-6.367847	1.485302	1.028823
C	-7.705966	1.333028	0.576981
H	-7.934052	0.444703	-0.029007
C	-8.682052	2.268378	0.862154
H	-9.717992	2.132052	0.517297
C	-8.337678	3.433177	1.599826
C	-9.288281	4.444479	1.918478
H	-10.330544	4.317002	1.585489
C	-8.897116	5.563877	2.633166
H	-9.611228	6.360492	2.889339
C	-7.538697	5.662560	3.037916
H	-7.198806	6.540945	3.616444
N	-6.624102	4.746882	2.760969
C	-6.979267	3.641580	2.051562
C	-5.975119	2.646633	1.730494
O	-4.669847	2.729625	2.032493
C	-4.019330	3.870931	2.606050
H	-4.192832	4.784232	2.010564
H	-2.945572	3.615803	2.574588
H	-4.354435	4.044946	3.644910
C	0.017272	-6.057789	-0.347452
C	1.226077	-6.611435	0.173568
C	1.298651	-7.990576	0.464859
H	2.228655	-8.384396	0.892646
C	0.192963	-8.813471	0.214336
H	0.263820	-9.887705	0.443410
C	-0.991592	-8.286058	-0.322867
H	-1.853267	-8.939052	-0.525295
C	-1.071357	-6.912240	-0.594921
H	-1.994884	-6.477950	-1.006605
N	2.312276	-5.743882	0.357987
H	2.155228	-4.788180	0.027819
C	3.572491	-5.982679	0.874970
O	3.934094	-7.031389	1.399050
C	4.502560	-4.806413	0.668885
C	4.873707	-4.408458	-0.647946
H	4.413538	-4.918662	-1.508116
C	5.818119	-3.414827	-0.852979
H	6.119277	-3.125761	-1.870886
C	6.400682	-2.746560	0.262006
C	7.362749	-1.704570	0.125890
H	7.714334	-1.418616	-0.877492
C	7.819183	-1.046374	1.255980
H	8.546036	-0.224647	1.180618
C	7.307345	-1.433540	2.524078
H	7.641638	-0.901425	3.433672
N	6.433967	-2.414224	2.702172
C	5.987338	-3.088225	1.602922
C	5.031864	-4.151423	1.784888
O	4.529945	-4.473121	3.003570
C	5.433398	-4.972549	3.995134
H	5.857729	-5.944404	3.662819
H	4.827757	-5.136753	4.905817
H	6.237465	-4.240252	4.206010
C	3.256289	-1.468496	-4.533473
C	4.596707	-1.132290	-4.165882
C	5.631262	-1.243446	-5.120409
H	6.650084	-0.974775	-4.817367
C	5.337792	-1.680115	-6.419255
H	6.154353	-1.760752	-7.152900
C	4.026163	-2.014770	-6.789106
H	3.802915	-2.355341	-7.810896
C	2.996043	-1.908369	-5.842179
H	1.959849	-2.160609	-6.113697
N	4.807791	-0.682789	-2.856407
H	4.007380	-0.761628	-2.214791
C	5.882541	0.004766	-2.338213
O	6.973830	0.107742	-2.910005
C	5.621596	0.725026	-1.034793
C	6.547705	1.765611	-0.738457
H	7.375371	1.890394	-1.451779
C	6.420634	2.572345	0.375594
H	7.146012	3.374768	0.578402
C	5.310224	2.398602	1.248167
C	5.041331	3.260025	2.349819
H	5.751438	4.070050	2.579299
C	3.884640	3.088652	3.091527
H	3.641023	3.752265	3.934045
C	2.997257	2.036918	2.732984
H	2.053305	1.894870	3.289323
N	3.226830	1.193966	1.739305
C	4.356633	1.345991	0.993694
C	4.565412	0.469739	-0.134763
O	3.736387	-0.564508	-0.409682
C	3.057091	-1.324547	0.601673
H	3.681496	-1.421488	1.509750
H	2.895062	-2.320134	0.148643

H	2.096370	-0.850217	0.875961

Conformation 10.
Multiplicity: 2
Charge: 0
E(B97-3c) = -6287.340214950242 Hartree
E(M06/def2-TZVP) = -6287.333843592487 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -6285.150703789915 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -6285.330952676737 Hartree
E(PBEh-3c) = -6277.940909811078 Hartree
E(PM6) = 241.98631 Kcal/mol
E(PM7) = 118.77608 Kcal/mol
E(ωB97X-V/def2-TZVP) = -6289.231338142972 Hartree
E(GFN1-xTB) = -298.851199646975 Hartree
E(GFN2-xTB) = -290.678223864397 Hartree
E(GFN-FF) = -36.545262904680 Hartree

Coordinates:

Cu	0.970674	0.068310	1.805932
N	2.373890	1.400704	1.233409
N	2.221537	-1.457550	1.333613
N	-0.525622	-1.257833	2.117820
N	-0.286385	1.604701	2.254749
C	2.217522	2.757378	1.082544
C	3.456893	3.351766	0.610528
H	3.596610	4.415069	0.388018
C	4.375334	2.336787	0.543796
H	5.423731	2.389810	0.231061
C	3.686878	1.122178	0.945568
C	4.301710	-0.145216	1.031839
C	3.585419	-1.353266	1.172228
C	4.173507	-2.678465	1.095187
H	5.242252	-2.894299	1.007011
C	3.136267	-3.575506	1.130990
H	3.183872	-4.666739	1.064798
C	1.922119	-2.802877	1.313473
C	0.641849	-3.366133	1.495993
C	-0.488393	-2.615960	1.888322
C	-1.777537	-3.207614	2.199772
H	-2.017830	-4.272454	2.108585
C	-2.584785	-2.188085	2.637982
H	-3.626441	-2.241289	2.971047
C	-1.787230	-0.974644	2.592760
C	-2.271736	0.295978	2.968021
C	-1.543219	1.494849	2.812685
C	-2.093406	2.815491	3.053813
H	-3.066057	3.013127	3.518152
C	-1.186083	3.718761	2.552584
H	-1.259956	4.811034	2.524477
C	-0.060555	2.949957	2.055956
C	1.074216	3.505083	1.428038
C	5.788954	-0.192531	0.959985
C	6.599526	0.475024	1.924843
C	8.004682	0.441116	1.792916
H	8.612999	0.956284	2.551917
C	8.618249	-0.233114	0.731730
H	9.715459	-0.240043	0.649870
C	7.828551	-0.898118	-0.218877
H	8.296461	-1.424075	-1.064075
C	6.433951	-0.871909	-0.096529
H	5.806069	-1.357674	-0.857828
N	6.069967	1.254045	2.983423
H	6.432201	2.210178	3.055632
C	4.998999	1.066623	3.850371
O	4.551383	2.021328	4.481821
C	4.524878	-0.338967	4.087044
C	5.465557	-1.397295	4.253787
H	6.532920	-1.185235	4.096174
C	5.061127	-2.664317	4.637421
H	5.798398	-3.468910	4.780442
C	3.682986	-2.936615	4.866642
C	3.193615	-4.203959	5.291602
H	3.905080	-5.028198	5.458098
C	1.833105	-4.378853	5.488149
H	1.421179	-5.343825	5.818510
C	0.958833	-3.282171	5.239608
H	-0.131790	-3.412765	5.361954
N	1.370860	-2.085382	4.853609
C	2.709208	-1.891014	4.676901
C	3.159054	-0.584291	4.284721
O	2.245493	0.382797	4.005626
C	1.585798	1.014371	5.112793
H	1.040677	0.265220	5.721503
H	0.864785	1.723465	4.667229
H	2.335213	1.568640	5.712818
C	0.487247	-4.847462	1.344786
C	-0.230010	-5.404924	0.246648
C	-0.357275	-6.808819	0.135363
H	-0.907561	-7.212460	-0.721876
C	0.217966	-7.645388	1.099192
H	0.106865	-8.735442	0.994261
C	0.928076	-7.108192	2.182819
H	1.378990	-7.765527	2.941248
C	1.055685	-5.717178	2.293746
H	1.601213	-5.275777	3.138744
N	-0.785153	-4.525653	-0.697528
H	-0.607043	-3.531438	-0.526460
C	-1.532603	-4.826697	-1.823544
O	-1.798056	-5.967544	-2.197920
C	-2.036103	-3.615525	-2.564912
C	-2.813064	-2.612029	-1.915314
H	-2.979537	-2.683840	-0.828153
C	-3.395146	-1.583213	-2.640861
H	-4.033874	-0.829751	-2.154917
C	-3.192491	-1.502700	-4.050127
C	-3.746687	-0.464098	-4.851537
H	-4.378237	0.310671	-4.390711
C	-3.464800	-0.433749	-6.207403
H	-3.869273	0.363746	-6.848243
C	-2.640577	-1.450630	-6.761895
H	-2.407237	-1.437437	-7.842943
N	-2.115348	-2.442389	-6.058188
C	-2.379116	-2.487090	-4.720065
C	-1.800453	-3.547031	-3.942964
O	-0.927496	-4.427770	-4.504085
C	-1.471694	-5.398891	-5.404275
H	-2.155641	-6.076101	-4.850794
H	-0.612512	-5.981740	-5.786219
H	-1.990519	-4.905862	-6.251203
C	-3.690185	0.376674	3.437626
C	-4.714038	0.834796	2.556796
C	-6.058958	0.835709	2.988246
H	-6.831396	1.172423	2.287215
C	-6.376710	0.402720	4.281991
H	-7.429373	0.411391	4.603368
C	-5.376460	-0.040183	5.160674
H	-5.632002	-0.378349	6.175705
C	-4.042392	-0.054088	4.728753
H	-3.242131	-0.408599	5.395905
N	-4.327564	1.280422	1.281905
H	-3.317839	1.269401	1.114549
C	-5.103976	1.797977	0.260873
O	-6.333914	1.812664	0.264231
C	-4.299849	2.426684	-0.851737
C	-3.265322	3.364544	-0.558594
H	-2.980548	3.539060	0.490526
C	-2.642679	4.085608	-1.564293
H	-1.867565	4.825899	-1.320671
C	-3.020787	3.892336	-2.923865
C	-2.426648	4.601157	-4.008329
H	-1.619226	5.322313	-3.809015
C	-2.850771	4.339797	-5.300488
H	-2.406672	4.862162	-6.160498
C	-3.868895	3.369160	-5.505117
H	-4.216638	3.149852	-6.531508
N	-4.444921	2.684211	-4.528515
C	-4.043568	2.929167	-3.246884
C	-4.664364	2.187641	-2.182096
O	-5.537973	1.181972	-2.466319
C	-6.857295	1.558825	-2.885184
H	-7.377189	2.065857	-2.046473
H	-7.382163	0.617050	-3.131088
H	-6.813377	2.204512	-3.785699
C	1.054837	4.954332	1.066916
C	0.890406	5.324277	-0.303230
C	0.872736	6.693556	-0.654429
H	0.752849	6.958571	-1.710931
C	1.011969	7.672114	0.338752
H	0.995828	8.733355	0.046957
C	1.172313	7.316762	1.686454
H	1.286830	8.090171	2.460187
C	1.193850	5.959086	2.039183
H	1.333760	5.655917	3.087794
N	0.753824	4.287273	-1.235852
H	0.690785	3.331564	-0.853953
C	0.657273	4.359576	-2.607205
O	0.624699	5.428653	-3.233571
C	0.630094	3.039334	-3.336732
C	0.816596	3.128900	-4.748506
H	0.920266	4.144368	-5.157179
C	0.852503	2.012634	-5.560212
H	0.982673	2.111392	-6.648694
C	0.764287	0.713128	-4.984918
C	0.872261	-0.489702	-5.739314
H	0.959034	-0.428854	-6.835491
C	0.873046	-1.711025	-5.088527
H	0.918132	-2.662552	-5.634912
C	0.772133	-1.722522	-3.669991
H	0.809156	-2.686279	-3.132966
N	0.620264	-0.632891	-2.933368
C	0.593526	0.577205	-3.561468
C	0.447077	1.766761	-2.758046

O	0.184245	1.681000	-1.428114
C	-0.749538	0.708624	-0.927293
H	-1.493905	0.441153	-1.701592
H	-1.249287	1.193417	-0.069198
H	-0.223136	-0.205021	-0.597790

Conformation 13.
Multiplicity: 2
Charge: 0
E(B97-3c) = -6287.358944214261 Hartree
E(M06/def2-TZVP) = -6287.353695945651 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -6285.170642422631 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -6285.349504448347 Hartree
E(PBEh-3c) = -6277.946062151756 Hartree
E(PM6) = 251.10809 Kcal/mol
E(PM7) = 107.18458 Kcal/mol
E(ωB97X-V/def2-TZVP) = -6289.250479072040 Hartree
E(GFN1-xTB) = -298.866174704961 Hartree
E(GFN2-xTB) = -290.694557285923 Hartree
E(GFN-FF) = -36.567491303311 Hartree

Coordinates:

Cu	-0.216160	0.790513	-1.626642
N	-2.017265	-0.161644	-1.792499
N	0.728322	-0.906117	-2.189537
N	1.588024	1.710995	-1.366451
N	-1.157008	2.466939	-0.973839
C	-3.257925	0.373211	-1.515162
C	-4.293274	-0.609171	-1.766234
H	-5.366968	-0.427805	-1.643225
C	-3.655029	-1.761462	-2.155746
H	-4.094366	-2.729228	-2.418900
C	-2.233609	-1.472843	-2.156865
C	-1.230628	-2.428802	-2.417822
C	0.143722	-2.126228	-2.462691
C	1.165368	-3.117123	-2.741905
H	0.966178	-4.161917	-3.001911
C	2.373617	-2.482982	-2.624286
H	3.374969	-2.899210	-2.771915
C	2.088804	-1.104421	-2.266890
C	3.091788	-0.137463	-2.050385
C	2.831198	1.175921	-1.628092
C	3.859605	2.177634	-1.423438
H	4.931743	2.007513	-1.570399
C	3.219941	3.324777	-1.023589
H	3.655371	4.298279	-0.773761
C	1.801440	3.019582	-0.990786
C	0.808440	3.949190	-0.623079
C	-0.567929	3.655040	-0.592151
C	-1.574387	4.577143	-0.100873
H	-1.367191	5.586771	0.269422
C	-2.780280	3.928066	-0.185118
H	-3.772306	4.293256	0.100385
C	-2.509656	2.615039	-0.740879
C	-3.507954	1.654084	-0.991343
C	-1.632095	-3.870388	-2.465955
C	-1.359939	-4.697555	-1.328877
C	-1.769996	-6.048302	-1.333437
H	-1.554103	-6.658587	-0.447988
C	-2.427679	-6.574090	-2.453565
H	-2.738532	-7.629987	-2.444395
C	-2.690695	-5.774926	-3.576987
H	-3.202062	-6.196497	-4.454956
C	-2.292275	-4.428953	-3.572599
H	-2.481583	-3.786368	-4.445749
N	-0.663870	-4.113791	-0.264731
H	-0.480458	-3.103153	-0.349406
C	-0.031452	-4.701712	0.812568
O	-0.213831	-5.869817	1.172420
C	1.024286	-3.837477	1.465608
C	1.994941	-4.530813	2.245059
H	1.829604	-5.610627	2.375554
C	3.090593	-3.892145	2.798034
H	3.825678	-4.451537	3.396636
C	3.306322	-2.507597	2.544452
C	4.456187	-1.793256	2.986284
H	5.205016	-2.314717	3.603213
C	4.625874	-0.466623	2.621554
H	5.503478	0.110841	2.946853
C	3.634594	0.146466	1.805662
H	3.759315	1.192768	1.472874
N	2.535379	-0.472301	1.404654
C	2.343146	-1.769682	1.767499
C	1.153652	-2.443181	1.305875
O	0.178297	-1.779089	0.649230
C	-0.255589	-0.474159	1.078388
H	-0.141298	-0.374509	2.175194
H	-1.316970	-0.411597	0.783353
H	0.353200	0.315134	0.600138
C	4.484179	-0.535194	-2.430879
C	4.762641	-0.661668	-3.821587
C	5.979436	-1.213551	-4.252748
H	6.154647	-1.339374	-5.329225
C	6.942011	-1.591369	-3.303782
H	7.896424	-2.022317	-3.642458
C	6.700093	-1.414775	-1.931836
H	7.463086	-1.705083	-1.194066
C	5.470001	-0.894569	-1.496436
H	5.248163	-0.802497	-0.422244
N	3.747828	-0.238896	-4.711209
H	3.181953	0.550700	-4.372400
C	3.027220	-1.114547	-5.510882
O	3.509490	-2.147299	-5.970807
C	1.550255	-0.793566	-5.657856
C	0.775576	-1.850027	-6.217022
H	1.346990	-2.713195	-6.588680
C	-0.604408	-1.812981	-6.265542
H	-1.176557	-2.647642	-6.698454
C	-1.299645	-0.700413	-5.716328
C	-2.719300	-0.617097	-5.651486
H	-3.321616	-1.435201	-6.077322
C	-3.321716	0.471757	-5.043016
H	-4.415350	0.552946	-4.965118
C	-2.490989	1.479587	-4.485514
H	-2.940735	2.339573	-3.958070
N	-1.168629	1.448053	-4.537514
C	-0.556147	0.396519	-5.149663
C	0.885597	0.353837	-5.170229
O	1.639272	1.353579	-4.645455
C	1.272521	2.740940	-4.622605
H	0.761967	3.027430	-5.562432
H	2.231767	3.285985	-4.528338
H	0.612349	2.967549	-3.767835
C	1.249982	5.325820	-0.239120
C	1.846244	5.572411	1.031045
C	2.315937	6.870224	1.337914
H	2.793754	7.037044	2.309604
C	2.170547	7.905477	0.405927
H	2.539900	8.910024	0.662957
C	1.560065	7.677681	-0.836866
H	1.444786	8.495500	-1.563437
C	1.106131	6.388399	-1.148801
H	0.638441	6.180040	-2.123076
N	1.924296	4.498263	1.929422
H	1.375067	3.656057	1.700609
C	2.645276	4.421871	3.100031
O	3.352746	5.332898	3.537750
C	2.573314	3.099167	3.835638
C	3.596554	2.913173	4.813651
H	4.311593	3.740613	4.928709
C	3.678512	1.767242	5.578232
H	4.483129	1.640744	6.318817
C	2.725144	0.724946	5.401878
C	2.785246	-0.510021	6.106298
H	3.579334	-0.660205	6.854665
C	1.866916	-1.506313	5.821498
H	1.894432	-2.481983	6.327850
C	0.877422	-1.251202	4.835405
H	0.160178	-2.040889	4.564249
N	0.764976	-0.103247	4.184751
C	1.667692	0.885643	4.437085
C	1.601768	2.099581	3.661103
O	0.655070	2.236109	2.682758
C	-0.731403	2.284637	3.068519
H	-1.025388	1.358855	3.599570
H	-1.306832	2.381106	2.129158
H	-0.920521	3.173520	3.706833
C	-4.908577	2.022424	-0.614844
C	-5.396506	1.723744	0.688079
C	-6.665374	2.205773	1.080329
H	-7.013111	2.010232	2.101017
C	-7.449546	2.935642	0.178791
H	-8.437175	3.299365	0.500806
C	-6.991760	3.200450	-1.121382
H	-7.612187	3.770898	-1.828302
C	-5.721839	2.746841	-1.504862
H	-5.328621	2.972842	-2.507978
N	-4.596798	0.935247	1.537451
H	-3.970510	0.252428	1.092735
C	-4.638421	0.906380	2.916617
O	-5.324028	1.681856	3.587287
C	-3.778285	-0.131434	3.606834
C	-3.626632	0.070776	5.011584
H	-4.076177	0.988360	5.417839
C	-3.007472	-0.854902	5.827078
H	-2.923658	-0.684980	6.911191
C	-2.482843	-2.053179	5.266822
C	-1.858024	-3.071324	6.041871
H	-1.801653	-2.950485	7.135191
C	-1.320859	-4.183548	5.412912
H	-0.834025	-4.986896	5.985297
C	-1.389188	-4.264530	3.993855

H	-0.935692	-5.116815	3.455793
N	-1.982435	-3.347427	3.241661
C	-2.557342	-2.268056	3.843077
C	-3.251389	-1.299940	3.023780
O	-3.390060	-1.478676	1.684549
C	-3.718815	-2.772733	1.138430
H	-2.803323	-3.313149	0.843631
H	-4.352660	-2.568332	0.256812
H	-4.277426	-3.376541	1.878610

Conformation 17.
Multiplicity: 2
Charge: 0
E(B97-3c) = -6287.319172005627 Hartree
E(M06/def2-TZVP) = -6287.313392255152 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -6285.129449916969 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -6285.304824974927 Hartree
E(PBEh-3c) = -6277.919914744156 Hartree
E(PM6) = 237.59374 Kcal/mol
E(PM7) = 132.12321 Kcal/mol
E(ωB97X-V/def2-TZVP) = -6289.202259619319 Hartree
E(GFN1-xTB) = -298.827719399502 Hartree
E(GFN2-xTB) = -290.672718880042 Hartree
E(GFN-FF) = -36.522153968158 Hartree

Coordinates:

Cu	-0.607665	-1.667057	0.309080
N	1.199236	-2.570075	0.423020
N	-0.497958	-1.693652	-1.712324
N	-2.364020	-0.675096	0.204498
N	-0.755423	-1.722828	2.332749
C	1.850344	-2.986794	1.565238
C	3.179280	-3.466082	1.232781
H	3.910142	-3.830433	1.962145
C	3.310237	-3.361333	-0.129132
H	4.160440	-3.637279	-0.761311
C	2.063324	-2.818278	-0.625969
C	1.776233	-2.652936	-1.991926
C	0.545345	-2.170826	-2.478262
C	0.201594	-2.107449	-3.884764
H	0.853261	-2.432607	-4.703192
C	-1.066939	-1.584091	-3.956830
H	-1.679120	-1.404964	-4.848446
C	-1.480303	-1.300164	-2.595668
C	-2.673870	-0.629957	-2.262980
C	-3.055279	-0.327782	-0.940967
C	-4.238353	0.435687	-0.590031
H	-4.961206	0.842315	-1.304124
C	-4.253214	0.543732	0.776579
H	-4.985004	1.067752	1.399596
C	-3.082547	-0.159064	1.264468
C	-2.787822	-0.335469	2.632641
C	-1.731670	-1.134144	3.109451
C	-1.518697	-1.461600	4.506967
H	-2.142554	-1.115185	5.336769
C	-0.417499	-2.275592	4.559874
H	0.044994	-2.735573	5.439628
C	0.083515	-2.389156	3.203884
C	1.322170	-2.972415	2.872842
C	2.819394	-3.065425	-2.982978
C	2.843013	-4.398858	-3.479223
C	3.829866	-4.761826	-4.421984
H	3.830755	-5.772059	-4.849208
C	4.795497	-3.834125	-4.829651
H	5.558095	-4.142576	-5.560707
C	4.783334	-2.521117	-4.334495
H	5.537401	-1.791104	-4.663004
C	3.785823	-2.144678	-3.424304
H	3.748164	-1.117571	-3.030979
N	1.836141	-5.275204	-3.046733
H	0.985658	-4.831304	-2.682173
C	1.745346	-6.656584	-3.020898
O	0.669886	-7.201061	-2.779195
C	2.974904	-7.478798	-3.297313
C	2.888634	-8.461134	-4.319344
H	1.945145	-8.535733	-4.879942
C	3.950201	-9.302602	-4.603475
H	3.879577	-10.052499	-5.405626
C	5.151355	-9.197676	-3.849690
C	6.297165	-10.002299	-4.110195
H	6.248610	-10.754887	-4.913081
C	7.449783	-9.824368	-3.364185
H	8.350643	-10.428710	-3.546656
C	7.449574	-8.831654	-2.346266
H	8.361305	-8.664657	-1.743731
N	6.403788	-8.073178	-2.058747
C	5.256933	-8.232841	-2.777799
C	4.121652	-7.387654	-2.489165
O	4.098485	-6.457260	-1.509897
C	4.784309	-6.643551	-0.267464
H	4.760615	-7.706099	0.046513
H	4.231634	-6.025399	0.465842
H	5.840492	-6.323825	-0.335291
C	-3.526226	-0.083620	-3.362031
C	-3.073005	1.041693	-4.104461
C	-3.932874	1.662400	-5.032770
H	-3.564769	2.534410	-5.592046
C	-5.227327	1.169735	-5.236043
H	-5.889407	1.665947	-5.961402
C	-5.669630	0.035759	-4.535348
H	-6.679408	-0.365056	-4.707959
C	-4.820524	-0.582024	-3.606289
H	-5.164377	-1.456146	-3.033210
N	-1.765243	1.530033	-3.902012
H	-1.000469	0.845810	-3.884623
C	-1.342030	2.835037	-3.720627
O	-0.140330	3.103793	-3.750935
C	-2.394531	3.833791	-3.326762
C	-3.213746	3.542018	-2.203426
H	-3.153988	2.541970	-1.752516
C	-4.016905	4.508208	-1.623760
H	-4.598385	4.285882	-0.715907
C	-4.028833	5.820995	-2.168676
C	-4.774977	6.880772	-1.581043
H	-5.347192	6.678584	-0.663002
C	-4.755679	8.139143	-2.156422
H	-5.315450	8.978797	-1.718740
C	-3.985350	8.331961	-3.334326
H	-3.964555	9.325772	-3.818859
N	-3.264313	7.380850	-3.907418
C	-3.250762	6.138045	-3.346797
C	-2.428940	5.103001	-3.929060
O	-1.710613	5.217631	-5.066535
C	-1.228547	6.454463	-5.585849
H	-2.028488	7.030487	-6.088216
H	-0.437644	6.173355	-6.308973
H	-0.799413	7.088425	-4.786186
C	-3.676629	0.343136	3.621802
C	-3.674875	1.756277	3.726586
C	-4.569059	2.399632	4.601457
H	-4.558845	3.496967	4.653777
C	-5.450658	1.651472	5.390701
H	-6.145565	2.164990	6.071927
C	-5.442843	0.249614	5.312742
H	-6.134390	-0.344379	5.928794
C	-4.562672	-0.395025	4.433701
H	-4.570310	-1.491619	4.344372
N	-2.792329	2.532308	2.925358
H	-1.775902	2.378638	3.009488
C	-3.258953	3.423729	1.982264
O	-4.465079	3.640067	1.811437
C	-2.205086	4.062802	1.129933
C	-1.258581	3.200643	0.491284
H	-1.276503	2.129746	0.745456
C	-0.398011	3.654852	-0.489372
H	0.282022	2.966386	-1.011444
C	-0.426914	5.026571	-0.874648
C	0.404234	5.558449	-1.901161
H	1.060824	4.876846	-2.459364
C	0.324406	6.908327	-2.202927
H	0.954110	7.354537	-2.987272
C	-0.593927	7.717471	-1.479997
H	-0.669848	8.796503	-1.710011
N	-1.394147	7.259599	-0.529122
C	-1.333547	5.934119	-0.226754
C	-2.235538	5.429649	0.789794
O	-3.026134	6.377402	1.328857
C	-3.615851	6.254809	2.614170
H	-4.583635	5.717074	2.569495
H	-3.761569	7.288846	2.982169
H	-2.946967	5.710249	3.316735
C	2.148000	-3.591793	3.953491
C	2.789898	-2.801608	4.953339
C	3.604485	-3.439841	5.918592
H	4.098758	-2.817457	6.672288
C	3.768017	-4.830106	5.896316
H	4.404930	-5.303513	6.659111
C	3.135542	-5.615004	4.920765
H	3.262810	-6.707539	4.907679
C	2.335664	-4.987237	3.956851
H	1.832566	-5.580581	3.178401
N	2.579715	-1.414632	4.934382
H	1.929333	-1.042794	4.225190
C	3.043297	-0.474403	5.826046
O	3.820237	-0.724517	6.751745
C	2.520312	0.940012	5.646230
C	2.976677	1.846827	6.649745
H	3.646870	1.421731	7.410529
C	2.620860	3.178521	6.652033
H	3.005575	3.864357	7.422114
C	1.740685	3.679236	5.653170
C	1.331076	5.040491	5.602640

H	1.719744	5.744416	6.355186
C	0.459019	5.453669	4.610932
H	0.131067	6.499947	4.526268
C	-0.029068	4.485494	3.694894
H	-0.742142	4.784606	2.908568
N	0.315916	3.203784	3.711133
C	1.220941	2.786170	4.646679
C	1.664886	1.412902	4.634588
O	1.215452	0.558084	3.664136
C	1.524354	0.867698	2.289982
H	1.063926	1.828622	1.991996
H	1.094370	0.038779	1.698455
H	2.624784	0.899788	2.143284

Conformation 22.
Multiplicity: 2
Charge: 0
E(B97-3c) = -6287.329015287301 Hartree
E(M06/def2-TZVP) = -6287.318642663349 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -6285.142703178262 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -6285.317520040165 Hartree
E(PBEh-3c) = -6277.926779512231 Hartree
E(PM6) = 254.54567 Kcal/mol
E(PM7) = 114.14864 Kcal/mol
E(ωB97X-V/def2-TZVP) = -6289.213333313693 Hartree
E(GFN1-xTB) = -298.845811164812 Hartree
E(GFN2-xTB) = -290.683398326237 Hartree
E(GFN-FF) = -36.536953511415 Hartree

Coordinates:

Cu	1.764629	-1.413395	-2.297578
N	1.382508	-2.792965	-0.850867
N	3.524999	-0.961011	-1.405539
N	2.121231	-0.004759	-3.715360
N	0.001077	-1.862165	-3.187042
C	0.295713	-3.640541	-0.780992
C	0.363552	-4.439548	0.426138
H	-0.366512	-5.204616	0.710437
C	1.483618	-4.035104	1.106733
H	1.859329	-4.400961	2.067884
C	2.122802	-3.016741	0.292614
C	3.327723	-2.372352	0.632402
C	3.986678	-1.450298	-0.201678
C	5.274151	-0.862937	0.115899
H	5.870326	-1.100337	1.004406
C	5.580142	-0.003280	-0.909932
H	6.468319	0.625025	-1.032909
C	4.477476	-0.066445	-1.848375
C	4.382452	0.746436	-2.995065
C	3.254841	0.774592	-3.837605
C	3.096095	1.719136	-4.926356
H	3.855580	2.444390	-5.238150
C	1.837855	1.525534	-5.436483
H	1.348842	2.062934	-6.255114
C	1.247385	0.428239	-4.691116
C	-0.021181	-0.120990	-4.968111
C	-0.557187	-1.231618	-4.281653
C	-1.819740	-1.857733	-4.626382
H	-2.470362	-1.555008	-5.453598
C	-2.026722	-2.859483	-3.715920
H	-2.877664	-3.542849	-3.640600
C	-0.887892	-2.853998	-2.817908
C	-0.770509	-3.703675	-1.701722
C	3.889631	-2.620362	1.993947
C	3.740156	-1.620104	2.992701
C	4.158056	-1.882687	4.312072
H	4.032810	-1.103953	5.077083
C	4.722825	-3.119671	4.644210
H	5.040226	-3.310586	5.680162
C	4.902412	-4.101126	3.656452
H	5.362577	-5.067400	3.910509
C	4.489304	-3.845725	2.341170
H	4.612301	-4.611239	1.560440
N	3.175396	-0.370281	2.644007
H	3.516439	0.074299	1.784220
C	2.189622	0.359929	3.287156
O	1.961419	1.523345	2.943615
C	1.363095	-0.386603	4.293025
C	0.825802	-1.636464	3.841727
H	1.094824	-1.982460	2.833669
C	-0.043433	-2.389614	4.599233
H	-0.458223	-3.330330	4.208522
C	-0.439343	-1.920504	5.883552
C	-1.331177	-2.638321	6.727784
H	-1.729702	-3.605542	6.384034
C	-1.694799	-2.101986	7.951886
H	-2.384075	-2.629703	8.627878
C	-1.158624	-0.837561	8.321056
H	-1.441545	-0.387009	9.290698
N	-0.319123	-0.140889	7.568568
C	0.050042	-0.657706	6.365476
C	0.978398	0.111872	5.551684
O	1.395309	1.241267	6.148290
C	2.558804	1.945706	5.745557
H	3.392041	1.248613	5.505620
H	2.849307	2.569676	6.611787
H	2.367823	2.577269	4.855828
C	5.477486	1.737847	-3.233639
C	5.293641	3.091428	-2.826178
C	6.343513	4.021098	-2.993195
H	6.185997	5.052273	-2.655239
C	7.551654	3.607546	-3.569694
H	8.361232	4.342668	-3.695101
C	7.739414	2.279308	-3.982559
H	8.690461	1.963147	-4.435753
C	6.700847	1.352649	-3.807349
H	6.828747	0.304214	-4.116413
N	4.050922	3.436519	-2.277242
H	3.367703	2.675474	-2.238871
C	3.605271	4.656801	-1.795555
O	4.299352	5.660773	-1.687817
C	2.126627	4.641790	-1.478648
C	1.197011	4.395349	-2.523093
H	1.582099	4.122691	-3.518374
C	-0.169042	4.514735	-2.316496
H	-0.881782	4.350678	-3.139433
C	-0.650809	4.892273	-1.033690
C	-2.029762	5.139207	-0.775408
H	-2.755605	5.025718	-1.595672
C	-2.440434	5.526512	0.488619
H	-3.498547	5.729555	0.710117
C	-1.457560	5.653130	1.506759
H	-1.761694	5.939269	2.530257
N	-0.165540	5.440434	1.311102
C	0.268090	5.081742	0.069365
C	1.686811	4.936158	-0.173406
O	2.653677	5.113137	0.743051
C	2.490965	4.795272	2.130631
H	1.823318	5.512812	2.640106
H	3.512920	4.843883	2.552930
H	2.100037	3.764174	2.254106
C	-0.852721	0.497387	-6.043270
C	-2.092141	1.118122	-5.718124
C	-2.901024	1.646899	-6.745792
H	-3.864005	2.099700	-6.483397
C	-2.478727	1.575731	-8.078802
H	-3.121292	1.992481	-8.869048
C	-1.249762	0.983059	-8.409096
H	-0.921211	0.924903	-9.457256
C	-0.447205	0.449993	-7.391902
H	0.506448	-0.041572	-7.636326
N	-2.493256	1.178038	-4.369897
H	-1.752698	1.023255	-3.680940
C	-3.791344	0.918877	-3.919989
O	-4.747524	0.797248	-4.674575
C	-3.908413	0.859824	-2.420881
C	-3.407299	1.930689	-1.636824
H	-2.833575	2.722018	-2.142263
C	-3.652676	2.014250	-0.275333
H	-3.267157	2.853611	0.319632
C	-4.440363	1.013479	0.350639
C	-4.827289	1.094860	1.719933
H	-4.485930	1.954500	2.317144
C	-5.621468	0.107096	2.272665
H	-5.936766	0.146708	3.324668
C	-5.996408	-0.994166	1.455186
H	-6.588319	-1.822469	1.883828
N	-5.654440	-1.111780	0.182726
C	-4.907492	-0.131236	-0.399119
C	-4.600668	-0.211071	-1.810904
O	-4.927942	-1.222013	-2.631175
C	-5.464280	-2.477974	-2.214733
H	-4.831470	-2.956722	-1.443487
H	-5.474762	-3.095437	-3.133868
H	-6.486860	-2.374978	-1.808054
C	-1.855657	-4.707730	-1.474391
C	-2.805348	-4.549064	-0.421559
C	-3.816689	-5.524335	-0.252550
H	-4.531052	-5.391710	0.567255
C	-3.884717	-6.625370	-1.114660
H	-4.681548	-7.370097	-0.965834
C	-2.958795	-6.784493	-2.156710
H	-3.014852	-7.651340	-2.831428
C	-1.953500	-5.823074	-2.326872
H	-1.213354	-5.928696	-3.134440
N	-2.698085	-3.417228	0.396212
H	-2.042958	-2.679262	0.103898
C	-3.319272	-3.183454	1.607165
O	-4.146440	-3.956109	2.102651
C	-2.911887	-1.932702	2.351076
C	-3.434861	-1.867322	3.674300
H	-4.054744	-2.721033	3.982753

C	-3.177914	-0.811785	4.522945
H	-3.565078	-0.802300	5.552598
C	-2.393848	0.279238	4.064515
C	-2.083221	1.401122	4.883645
H	-2.422900	1.407152	5.930684
C	-1.346128	2.450412	4.362885
H	-1.076379	3.321392	4.977554
C	-0.927288	2.375580	3.007635
H	-0.353705	3.206376	2.564236
N	-1.180546	1.340063	2.222294
C	-1.875543	0.281594	2.717879
C	-2.111488	-0.870075	1.872270
O	-1.624316	-0.987654	0.611228
C	-0.666400	-0.118040	-0.015919
H	-1.105882	0.873036	-0.221723
H	-0.404239	-0.637334	-0.956798
H	0.233525	0.013041	0.613544

Conformation 26.
Multiplicity: 2
Charge: 0
E(B97-3c) = -6287.318670069100 Hartree
E(M06/def2-TZVP) = -6287.311337184255 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -6285.132064212398 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -6285.306367682145 Hartree
E(PBEh-3c) = -6277.913089849062 Hartree
E(PM6) = 266.17446 Kcal/mol
E(PM7) = 138.11293 Kcal/mol
E(ωB97X-V/def2-TZVP) = -6289.203175746834 Hartree
E(GFN1-xTB) = -298.825300793360 Hartree
E(GFN2-xTB) = -290.669636716637 Hartree
E(GFN-FF) = -36.519877367473 Hartree

Coordinates:

Cu	0.270814	-0.816000	-0.240811
N	1.778401	-1.921312	0.543756
N	-0.748985	-2.509735	-0.670652
N	-1.219292	0.296347	-1.046881
N	1.292135	0.890775	0.201939
C	2.917334	-1.446658	1.159822
C	3.773790	-2.551358	1.543316
H	4.750472	-2.443180	2.025624
C	3.123723	-3.699622	1.172729
H	3.464910	-4.735001	1.276558
C	1.862863	-3.297700	0.581245
C	0.868426	-4.198484	0.159927
C	-0.349733	-3.804678	-0.425008
C	-1.391443	-4.731507	-0.822987
H	-1.341859	-5.818790	-0.714089
C	-2.421534	-3.979611	-1.320457
H	-3.379618	-4.323378	-1.723664
C	-2.018993	-2.591373	-1.202897
C	-2.849300	-1.508685	-1.554295
C	-2.453941	-0.160296	-1.466637
C	-3.298028	0.959267	-1.832199
H	-4.336845	0.869789	-2.167038
C	-2.544565	2.095171	-1.670197
H	-2.822790	3.137007	-1.856740
C	-1.253207	1.670566	-1.173834
C	-0.226402	2.569359	-0.819471
C	0.946958	2.182988	-0.142638
C	1.935521	3.113688	0.368790
H	1.912795	4.197817	0.219999
C	2.852434	2.372763	1.068496
H	3.736678	2.722249	1.611788
C	2.462465	0.984163	0.929124
C	3.230150	-0.095768	1.405338
C	1.098957	-5.658082	0.368618
C	1.203770	-6.239854	1.661490
C	1.483078	-7.616991	1.787691
H	1.554251	-8.049900	2.797514
C	1.650744	-8.427328	0.659844
H	1.869425	-9.498522	0.783411
C	1.524575	-7.868435	-0.621113
H	1.649798	-8.493429	-1.517618
C	1.250891	-6.501526	-0.753229
H	1.173094	-6.048874	-1.752932
N	1.108962	-5.481066	2.853061
H	1.809988	-5.687201	3.567786
C	0.173156	-4.520125	3.207534
O	-0.795147	-4.207276	2.530094
C	0.494116	-3.915982	4.559452
C	0.384305	-4.698763	5.739730
H	0.049321	-5.744161	5.650386
C	0.651405	-4.160728	6.989826
H	0.537332	-4.766572	7.901496
C	1.095063	-2.814060	7.097100
C	1.431381	-2.202409	8.338516
H	1.317036	-2.781013	9.269090
C	1.908868	-0.902182	8.358864
H	2.180391	-0.405844	9.302185
C	2.062683	-0.216168	7.122055
H	2.473612	0.809774	7.108960
N	1.741935	-0.738421	5.947774
C	1.244091	-2.006774	5.908326
C	0.889871	-2.572118	4.629882
O	1.012766	-1.897456	3.471909
C	0.439587	-0.585518	3.329839
H	-0.558377	-0.562969	3.809539
H	0.320665	-0.439481	2.240691
H	1.105856	0.193464	3.743875
C	-4.232613	-1.820066	-2.025113
C	-5.187396	-2.377921	-1.123424
C	-6.476172	-2.714974	-1.596029
H	-7.186851	-3.166703	-0.894863
C	-6.815063	-2.479019	-2.934363
H	-7.823893	-2.746169	-3.284666
C	-5.889358	-1.911503	-3.823595
H	-6.159432	-1.731632	-4.874753
C	-4.605366	-1.589052	-3.361948
H	-3.856194	-1.163628	-4.046716
N	-4.795784	-2.553333	0.209844
H	-3.899157	-2.133383	0.499393
C	-5.407463	-3.303801	1.187616
O	-6.447708	-3.945287	1.015521
C	-4.728163	-3.304957	2.542547
C	-5.258313	-4.263274	3.457431
H	-6.045158	-4.922769	3.063977
C	-4.826192	-4.344420	4.764176
H	-5.240841	-5.098700	5.450445
C	-3.851369	-3.426383	5.246413
C	-3.393772	-3.423572	6.593154
H	-3.794635	-4.172719	7.294117
C	-2.464666	-2.481891	7.002391
H	-2.090080	-2.448503	8.035508
C	-1.995829	-1.542047	6.047541
H	-1.262496	-0.773168	6.350086
N	-2.381814	-1.523388	4.780118
C	-3.293748	-2.441150	4.353349
C	-3.720884	-2.423576	2.974227
O	-3.105887	-1.602308	2.070439
C	-3.190715	-0.175033	2.219485
H	-4.222912	0.172392	1.996964
H	-2.490918	0.244406	1.472804
H	-2.887862	0.129187	3.238344
C	-0.439105	4.022295	-1.104667
C	-0.392302	4.524246	-2.437120
C	-0.545716	5.910713	-2.655920
H	-0.444764	6.315234	-3.669776
C	-0.799913	6.777577	-1.587279
H	-0.922102	7.852850	-1.786814
C	-0.878978	6.287147	-0.275337
H	-1.080315	6.966247	0.566109
C	-0.683566	4.919142	-0.046392
H	-0.728031	4.514727	0.975961
N	-0.143546	3.616338	-3.483558
H	0.321112	2.739199	-3.215784
C	-0.485794	3.635963	-4.819075
O	-0.131088	2.727536	-5.573407
C	-1.259390	4.801942	-5.377959
C	-0.614292	5.605663	-6.355001
H	0.429435	5.370320	-6.611758
C	-1.271660	6.656953	-6.971308
H	-0.762235	7.282390	-7.719735
C	-2.624176	6.935999	-6.632780
C	-3.352367	8.020552	-7.199831
H	-2.859500	8.659010	-7.950013
C	-4.655388	8.261398	-6.798693
H	-5.240154	9.093965	-7.216891
C	-5.231148	7.403937	-5.821381
H	-6.266898	7.582286	-5.478490
N	-4.597911	6.376124	-5.279073
C	-3.315685	6.117013	-5.662069
C	-2.608882	5.013430	-5.056838
O	-3.143824	4.181575	-4.135028
C	-4.520268	3.790266	-4.176554
H	-5.167314	4.527506	-3.667131
H	-4.560652	2.808749	-3.666718
H	-4.871454	3.677407	-5.221538
C	4.456162	0.188899	2.213790
C	5.643260	0.692058	1.604242
C	6.791838	0.909740	2.400176
H	7.697143	1.288007	1.911911
C	6.751674	0.642559	3.774810
H	7.655365	0.820229	4.378147
C	5.583983	0.154767	4.381734
H	5.554647	-0.051302	5.462343
C	4.444783	-0.073404	3.596286
H	3.519754	-0.453332	4.057888
N	5.599011	0.958819	0.230583
H	4.701814	0.786356	-0.251250
C	6.553881	1.552305	-0.563563

O	7.695242	1.830245	-0.183839
C	6.105931	1.912407	-1.968558
C	7.080121	2.629770	-2.725483
H	8.044451	2.800290	-2.225265
C	6.832345	3.077117	-4.006969
H	7.604471	3.619085	-4.574450
C	5.556556	2.861069	-4.600223
C	5.208585	3.337683	-5.895376
H	5.966611	3.872358	-6.489658
C	3.927200	3.132176	-6.378136
H	3.625375	3.487731	-7.374646
C	2.984687	2.455430	-5.554606
H	1.942183	2.315761	-5.891533
N	3.274207	1.985881	-4.347719
C	4.538613	2.155008	-3.863576
C	4.852948	1.642414	-2.551794
O	3.911074	0.956397	-1.838352
C	3.295433	-0.212753	-2.415756
H	2.705972	0.067088	-3.307662
H	2.637956	-0.617943	-1.625566
H	4.072517	-0.963096	-2.676102

Conformation 3.
Multiplicity: 2
Charge: 0
E(B97-3c) = -6287.335305010298 Hartree
E(M06/def2-TZVP) = -6287.332416021612 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -6285.148760403490 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -6285.324726779480 Hartree
E(PBEh-3c) = -6277.930383103001 Hartree
E(PM6) = 239.99018 Kcal/mol
E(PM7) = 115.73053 Kcal/mol
E(ωB97X-V/def2-TZVP) = -6289.223305646209 Hartree
E(GFN1-xTB) = -298.850032310286 Hartree
E(GFN2-xTB) = -290.687291468786 Hartree
E(GFN-FF) = -36.548023991548 Hartree

Coordinates:

Cu	0.069978	-0.934022	2.242479
N	-0.110109	-1.710096	0.383162
N	-1.931641	-0.699416	2.351605
N	0.283768	-0.039429	4.047402
N	2.065958	-1.325237	2.204614
C	0.908565	-2.160676	-0.432491
C	0.384153	-2.490014	-1.744386
H	0.983296	-2.882464	-2.573651
C	-0.964502	-2.239516	-1.706015
H	-1.712838	-2.390049	-2.490304
C	-1.265152	-1.775098	-0.366355
C	-2.570415	-1.500498	0.090439
C	-2.859456	-1.043741	1.392031
C	-4.201136	-0.795112	1.888048
H	-5.122713	-1.010329	1.337577
C	-4.064600	-0.248319	3.138865
H	-4.849183	0.081673	3.828515
C	-2.641358	-0.163644	3.404910
C	-2.091554	0.511235	4.516269
C	-0.709299	0.591813	4.770339
C	-0.124811	1.346192	5.863988
H	-0.691008	1.961102	6.571142
C	1.228374	1.135996	5.810491
H	2.010691	1.558755	6.447806
C	1.471746	0.254415	4.685544
C	2.740787	-0.239425	4.332633
C	2.981037	-1.039860	3.197574
C	4.266369	-1.619926	2.864085
H	5.157161	-1.576249	3.499656
C	4.129271	-2.212648	1.634015
H	4.883190	-2.746560	1.046741
C	2.757209	-2.001858	1.218071
C	2.252984	-2.347011	-0.052424
C	-3.708191	-1.650170	-0.868852
C	-4.136043	-2.932212	-1.322139
C	-5.237801	-3.015995	-2.201566
H	-5.609114	-3.998535	-2.516135
C	-5.878754	-1.856749	-2.653234
H	-6.731415	-1.952006	-3.342628
C	-5.458550	-0.591047	-2.217188
H	-5.964844	0.321918	-2.563552
C	-4.388696	-0.502126	-1.318115
H	-4.055883	0.477328	-0.947733
N	-3.470244	-4.056807	-0.814021
H	-2.903727	-3.885409	0.024971
C	-3.412092	-5.386400	-1.193143
O	-2.884500	-6.212533	-0.449802
C	-4.015086	-5.830530	-2.499506
C	-4.955021	-6.894251	-2.436633
H	-5.219765	-7.283056	-1.442481
C	-5.517243	-7.432677	-3.580335
H	-6.254115	-8.247557	-3.519627
C	-5.138333	-6.926966	-4.853622
C	-5.699342	-7.408663	-6.070657
H	-6.440825	-8.222204	-6.029682
C	-5.316368	-6.848689	-7.277420
H	-5.736189	-7.198838	-8.231982
C	-4.360418	-5.796667	-7.259867
H	-4.045632	-5.326325	-8.209570
N	-3.802113	-5.328691	-6.155022
C	-4.159009	-5.867547	-4.954913
C	-3.572346	-5.344204	-3.742400
O	-2.647734	-4.357917	-3.710357
C	-1.679936	-4.178616	-4.749054
H	-1.306801	-5.153754	-5.120527
H	-0.846678	-3.620884	-4.279618
H	-2.097824	-3.615242	-5.602729
C	-3.016969	1.295492	5.394284
C	-3.605941	2.497219	4.892968
C	-4.462635	3.258557	5.716608
H	-4.902671	4.175406	5.306234
C	-4.729860	2.830417	7.023780
H	-5.400209	3.431660	7.656856
C	-4.153082	1.655197	7.529738
H	-4.366429	1.325929	8.557416
C	-3.299243	0.898782	6.712210
H	-2.838669	-0.026252	7.090415
N	-3.293092	2.851940	3.576365
H	-2.633134	2.219771	3.097631
C	-3.861808	3.801322	2.757361
O	-4.669803	4.655455	3.125630
C	-3.508206	3.628926	1.290880
C	-4.413422	4.240213	0.373818
H	-5.195099	4.878082	0.812415
C	-4.329876	4.017423	-0.987781
H	-5.042114	4.493974	-1.679078
C	-3.344575	3.130593	-1.508425
C	-3.250039	2.782880	-2.886196
H	-3.951299	3.237279	-3.603755
C	-2.296214	1.866463	-3.296436
H	-2.204517	1.564439	-4.349706
C	-1.430282	1.302015	-2.319083
H	-0.679531	0.548470	-2.617964
N	-1.463478	1.622249	-1.035547
C	-2.393762	2.521657	-0.611075
C	-2.458847	2.840844	0.790269
O	-1.510213	2.287436	1.613615
C	-0.502411	3.195756	2.102184
H	0.063887	3.623930	1.251229
H	0.181186	2.600000	2.734609
H	-0.955575	4.005201	2.713347
C	3.904299	0.077713	5.210880
C	4.999141	0.855305	4.748206
C	6.137209	1.016135	5.562417
H	6.970275	1.628320	5.185610
C	6.197829	0.433873	6.834757
H	7.095535	0.569273	7.456531
C	5.103124	-0.299598	7.317371
H	5.134184	-0.750788	8.320316
C	3.972040	-0.471575	6.508215
H	3.122424	-1.073021	6.864839
N	4.987348	1.472745	3.473869
H	5.737206	1.264860	2.804077
C	4.042262	2.381741	3.055820
O	3.092378	2.732295	3.762020
C	4.243758	2.980775	1.684781
C	3.527824	4.192327	1.458989
H	2.967811	4.591339	2.317095
C	3.503491	4.811230	0.226294
H	2.942037	5.744276	0.071072
C	4.187572	4.219707	-0.871598
C	4.163104	4.771492	-2.183393
H	3.585308	5.691912	-2.361715
C	4.840687	4.138447	-3.211463
H	4.823487	4.531358	-4.238071
C	5.548269	2.942027	-2.917685
H	6.072454	2.398667	-3.724097
N	5.602817	2.401303	-1.710394
C	4.937597	3.001745	-0.685021
C	4.974361	2.398148	0.628582
O	5.724513	1.303084	0.913908
C	5.974825	0.236228	-0.017681
H	5.062150	-0.002253	-0.594838
H	6.251744	-0.629726	0.611286
H	6.783798	0.499301	-0.720666
C	3.200528	-2.950680	-1.043218
C	3.695236	-2.199382	-2.151408
C	4.603191	-2.803741	-3.051384
H	4.969800	-2.207516	-3.894532
C	5.008208	-4.129943	-2.856472
H	5.715432	-4.582340	-3.568440
C	4.524199	-4.878333	-1.773184
H	4.839140	-5.921916	-1.625643
C	3.625107	-4.281753	-0.877878

H	3.227727	-4.851793	-0.024635
N	3.244370	-0.880488	-2.300375
H	2.659525	-0.501932	-1.543004
C	3.429102	-0.017652	-3.361245
O	4.146564	-0.269242	-4.334415
C	2.626331	1.265362	-3.324978
C	2.498981	1.899292	-4.591156
H	3.000068	1.399117	-5.432354
C	1.786546	3.069622	-4.759998
H	1.681169	3.532430	-5.752938
C	1.190107	3.694364	-3.632703
C	0.459417	4.911539	-3.736427
H	0.333389	5.371069	-4.729514
C	-0.075193	5.497241	-2.602113
H	-0.648299	6.434680	-2.651211
C	0.136654	4.852783	-1.354277
H	-0.274738	5.299883	-0.430316
N	0.803259	3.718285	-1.215597
C	1.326450	3.111387	-2.316388
C	2.037542	1.855222	-2.181562
O	2.222865	1.198211	-1.017973
C	1.539189	1.451606	0.227133
H	1.842385	2.423842	0.642076
H	1.874235	0.635794	0.891373
H	0.442456	1.411627	0.076391

Conformation 30.
Multiplicity: 2
Charge: 0
E(B97-3c) = -6287.335181890482 Hartree
E(M06/def2-TZVP) = -6287.329801195106 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -6285.146661111422 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -6285.325660216599 Hartree
E(PBEh-3c) = -6277.931148379664 Hartree
E(PM6) = 274.06109 Kcal/mol
E(PM7) = 124.90508 Kcal/mol
E(ωB97X-V/def2-TZVP) = -6289.224330992368 Hartree
E(GFN1-xTB) = -298.835888980236 Hartree
E(GFN2-xTB) = -290.671057223873 Hartree
E(GFN-FF) = -36.542369676091 Hartree

Coordinates:

Cu	-0.528735	0.006191	-0.045052
N	1.295766	0.865926	-0.179446
N	0.017308	-1.428416	-1.366172
N	-2.354582	-0.839779	0.091952
N	-1.047221	1.388506	1.352926
C	1.780578	1.933413	0.555729
C	3.096934	2.301938	0.077868
H	3.697460	3.125442	0.477211
C	3.413376	1.430641	-0.936371
H	4.329820	1.389651	-1.534851
C	2.296882	0.520206	-1.071150
C	2.308114	-0.623405	-1.898779
C	1.236219	-1.528507	-2.008587
C	1.270156	-2.723179	-2.828062
H	2.122323	-3.042577	-3.436290
C	0.049272	-3.329501	-2.691965
H	-0.299773	-4.250067	-3.170117
C	-0.721283	-2.525069	-1.761702
C	-2.030180	-2.850316	-1.334554
C	-2.784617	-2.026943	-0.476818
C	-4.161105	-2.280865	-0.099496
H	-4.734829	-3.166800	-0.387317
C	-4.575197	-1.204815	0.643502
H	-5.556889	-1.024523	1.093951
C	-3.434489	-0.321662	0.770271
C	-3.472738	0.899098	1.482810
C	-2.320739	1.633736	1.823244
C	-2.301610	2.730492	2.770569
H	-3.182045	3.131010	3.283793
C	-0.989426	3.103991	2.912860
H	-0.571978	3.877380	3.566173
C	-0.222426	2.310478	1.969320
C	1.118736	2.577885	1.624132
C	3.585830	-0.942926	-2.609238
C	4.702594	-1.407569	-1.856202
C	5.939619	-1.627905	-2.495362
H	6.793878	-1.954928	-1.891232
C	6.056812	-1.416169	-3.875538
H	7.026700	-1.592381	-4.364853
C	4.953352	-0.995678	-4.634422
H	5.049284	-0.839753	-5.719078
C	3.726422	-0.761573	-3.996316
H	2.857469	-0.406525	-4.571059
N	4.520702	-1.623770	-0.478189
H	3.545826	-1.729553	-0.190748
C	5.437746	-1.373751	0.533655
O	6.635511	-1.198112	0.323958
C	4.816438	-1.243397	1.903190
C	3.504095	-0.706621	2.061391
H	2.900826	-0.470820	1.174417
C	2.972244	-0.421266	3.305842
H	1.958796	-0.001063	3.392452
C	3.742418	-0.658668	4.476790
C	3.267359	-0.385893	5.790341
H	2.270308	0.064123	5.917756
C	4.060681	-0.703045	6.880671
H	3.723565	-0.511584	7.910046
C	5.331965	-1.299094	6.646603
H	5.971854	-1.572873	7.505375
N	5.816886	-1.559522	5.441587
C	5.057289	-1.237644	4.355612
C	5.577673	-1.543453	3.044837
O	6.743417	-2.215369	2.918858
C	7.957624	-1.520810	3.217395
H	8.126679	-0.730243	2.456871
H	8.766757	-2.271381	3.146690
H	7.935978	-1.100677	4.243244
C	-2.627771	-4.122773	-1.841618
C	-2.005476	-5.365688	-1.534514
C	-2.482351	-6.555468	-2.118107
H	-1.967908	-7.497677	-1.893122
C	-3.594408	-6.520438	-2.969272
H	-3.959786	-7.456029	-3.419622
C	-4.244754	-5.305790	-3.238022
H	-5.118793	-5.276903	-3.905676
C	-3.762268	-4.114279	-2.678495
H	-4.238704	-3.155424	-2.927989
N	-0.913944	-5.367969	-0.645455
H	-0.892554	-4.660822	0.102065
C	0.288244	-6.000618	-0.877230
O	0.460705	-6.791432	-1.807923
C	1.418727	-5.651597	0.067176
C	2.654549	-6.291753	-0.241269
H	2.645416	-6.939359	-1.129969
C	3.792098	-6.105903	0.517499
H	4.739238	-6.597309	0.248058
C	3.731391	-5.310689	1.695333
C	4.829562	-5.163856	2.589528
H	5.800639	-5.609627	2.324517
C	4.658804	-4.479033	3.779171
H	5.490043	-4.329092	4.482438
C	3.381370	-3.922532	4.059695
H	3.218277	-3.389102	5.012986
N	2.349855	-3.984674	3.232587
C	2.495818	-4.658631	2.055761
C	1.357345	-4.780016	1.174281
O	0.183226	-4.136286	1.434827
C	0.149498	-2.798648	1.958163
H	0.261552	-2.799830	3.055979
H	-0.828521	-2.382179	1.649783
H	0.963247	-2.187361	1.517703
C	-4.830389	1.499248	1.668259
C	-5.488877	1.918568	0.469056
C	-6.808825	2.402797	0.513297
H	-7.302324	2.680517	-0.426620
C	-7.460650	2.507424	1.750733
H	-8.492826	2.887818	1.784263
C	-6.811377	2.139412	2.940069
H	-7.330522	2.229130	3.905684
C	-5.501798	1.632707	2.893540
H	-4.998617	1.303415	3.815201
N	-4.753375	1.801171	-0.718251
H	-3.753257	1.658775	-0.561190
C	-5.169159	1.428990	-1.985385
O	-6.331405	1.473700	-2.379281
C	-3.996080	0.941538	-2.806245
C	-2.767206	1.669637	-2.811160
H	-2.726187	2.634186	-2.274695
C	-1.664292	1.202616	-3.504800
H	-0.719425	1.767167	-3.505380
C	-1.737762	-0.014162	-4.238542
C	-0.643847	-0.552772	-4.971025
H	0.316989	-0.014382	-4.974751
C	-0.802982	-1.747004	-5.653316
H	0.026247	-2.198658	-6.217062
C	-2.065912	-2.399246	-5.600958
H	-2.209580	-3.356495	-6.134325
N	-3.110179	-1.934783	-4.931701
C	-2.968700	-0.763453	-4.249913
C	-4.091916	-0.273183	-3.492342
O	-5.199648	-1.051441	-3.352505
C	-6.119137	-1.052394	-4.448664
H	-6.568373	-0.042993	-4.559489
H	-6.912675	-1.777647	-4.188379
H	-5.617884	-1.374990	-5.384895
C	1.881553	3.617998	2.385576
C	1.561816	5.006445	2.299157
C	2.326430	5.945234	3.029403
H	2.060397	7.005242	2.948277
C	3.394533	5.514545	3.825746

H	3.978201	6.261181	4.385567
C	3.726973	4.153992	3.906511
H	4.569985	3.815681	4.526869
C	2.971245	3.220954	3.184179
H	3.222353	2.151281	3.227666
N	0.491464	5.377876	1.476464
H	0.005563	4.617786	0.974813
C	-0.107769	6.609667	1.340888
O	0.287400	7.643288	1.884991
C	-1.352308	6.629438	0.474771
C	-2.090315	7.850600	0.520964
H	-1.673889	8.642762	1.159926
C	-3.257398	8.027233	-0.194335
H	-3.815118	8.974414	-0.135300
C	-3.756485	6.977549	-1.017098
C	-4.963245	7.073514	-1.765265
H	-5.550609	8.003930	-1.718545
C	-5.380065	5.997430	-2.531526
H	-6.310476	6.033919	-3.116566
C	-4.575854	4.825639	-2.553025
H	-4.893094	3.957291	-3.157912
N	-3.446215	4.696894	-1.872199
C	-3.026083	5.739599	-1.102662
C	-1.818684	5.585349	-0.336786
O	-1.175294	4.371049	-0.367808
C	-0.396986	4.080821	-1.539655
H	-1.022189	4.157524	-2.451114
H	-0.033577	3.044427	-1.412592
H	0.469345	4.773290	-1.613196

Conformation 6.
Multiplicity: 2
Charge: 0
E(B97-3c) = -6287.321627227346 Hartree
E(M06/def2-TZVP) = -6287.318295915039 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -6285.136873575140 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -6285.312063486670 Hartree
E(PBEh-3c) = -6277.916003702228 Hartree
E(PM6) = 257.39815 Kcal/mol
E(PM7) = 133.22851 Kcal/mol
E(ωB97X-V/def2-TZVP) = -6289.206697843812 Hartree
E(GFN1-xTB) = -298.825323984688 Hartree
E(GFN2-xTB) = -290.664448258978 Hartree
E(GFN-FF) = -36.528459760401 Hartree

Coordinates:

Cu	-0.237623	-1.069419	1.286095
N	0.064409	-3.073261	1.425940
N	-2.035995	-1.394530	0.420936
N	-0.573721	0.928870	1.230431
N	1.617973	-0.739924	2.036499
C	1.169510	-3.711399	1.952379
C	0.990788	-5.149617	1.889553
H	1.722619	-5.884974	2.238954
C	-0.234812	-5.372165	1.315792
H	-0.721938	-6.328143	1.097575
C	-0.794982	-4.070534	1.009094
C	-2.021169	-3.881594	0.344517
C	-2.561859	-2.613965	0.046467
C	-3.830688	-2.423824	-0.629598
H	-4.447919	-3.230577	-1.039096
C	-4.083789	-1.075821	-0.621609
H	-4.955844	-0.546885	-1.019967
C	-2.956238	-0.441911	0.035360
C	-2.852943	0.948070	0.243063
C	-1.729341	1.567891	0.823592
C	-1.573346	3.003089	0.956753
H	-2.348913	3.738300	0.717186
C	-0.297650	3.221591	1.416033
H	0.192428	4.173237	1.647572
C	0.325313	1.923027	1.556394
C	1.671324	1.738579	1.927370
C	2.253212	0.478640	2.159361
C	3.612305	0.287762	2.632124
H	4.335595	1.091381	2.803380
C	3.774830	-1.057821	2.831995
H	4.657793	-1.590029	3.201691
C	2.532424	-1.692648	2.435839
C	2.340878	-3.087164	2.425048
C	-2.831707	-5.089082	-0.008531
C	-3.987998	-5.411023	0.762510
C	-4.760559	-6.543933	0.426029
H	-5.647463	-6.769482	1.029711
C	-4.383726	-7.344763	-0.660074
H	-4.996422	-8.223710	-0.912210
C	-3.243019	-7.042441	-1.419553
H	-2.953010	-7.676443	-2.270290
C	-2.475012	-5.916913	-1.086772
H	-1.581910	-5.656514	-1.674686
N	-4.300805	-4.565563	1.836786
H	-3.622955	-3.815617	1.996996
C	-5.437868	-4.519883	2.629429
O	-6.324894	-5.374165	2.606005
C	-5.514583	-3.271404	3.468527
C	-5.296998	-2.029695	2.787832
H	-4.981147	-2.059811	1.734380
C	-5.529624	-0.804770	3.379221
H	-5.379118	0.125486	2.810948
C	-6.000383	-0.752704	4.721702
C	-6.281164	0.466522	5.400205
H	-6.140839	1.420270	4.867030
C	-6.724217	0.433199	6.712004
H	-6.951011	1.357263	7.264636
C	-6.877577	-0.832595	7.341765
H	-7.223361	-0.880895	8.391260
N	-6.626464	-1.989591	6.748441
C	-6.203628	-1.974113	5.456220
C	-5.938508	-3.251562	4.813446
O	-6.104812	-4.305501	5.625260
C	-5.509790	-5.570157	5.371663
H	-6.114966	-6.169559	4.663797
H	-5.445844	-6.076225	6.353590
H	-4.485989	-5.453568	4.952615
C	-3.980001	1.814134	-0.219789
C	-4.211276	2.036612	-1.611040
C	-5.300034	2.849539	-2.006012
H	-5.469416	3.002235	-3.077810
C	-6.129449	3.435058	-1.041548
H	-6.970809	4.062698	-1.372863
C	-5.899930	3.232725	0.327740
H	-6.553938	3.694363	1.082099
C	-4.825801	2.424117	0.724645
H	-4.623451	2.249694	1.792803
N	-3.335252	1.439788	-2.525982
H	-2.540280	0.897713	-2.147927
C	-3.398875	1.443207	-3.903724
O	-4.287454	2.000012	-4.553602
C	-2.283832	0.703033	-4.618895
C	-2.431286	0.645149	-6.038004
H	-3.338361	1.112421	-6.447852
C	-1.481561	0.061039	-6.850969
H	-1.613429	0.037409	-7.943565
C	-0.313548	-0.519043	-6.279006
C	0.709046	-1.137787	-7.051815
H	0.609171	-1.164655	-8.148380
C	1.807895	-1.693756	-6.417110
H	2.617658	-2.174732	-6.985155
C	1.868863	-1.638945	-4.998351
H	2.731595	-2.082335	-4.466882
N	0.939064	-1.074722	-4.243168
C	-0.139446	-0.501351	-4.848828
C	-1.144134	0.131010	-4.027601
O	-1.001009	0.128051	-2.669250
C	0.113547	0.874799	-2.125672
H	1.073870	0.497054	-2.517945
H	0.073049	0.713206	-1.034907
H	0.002900	1.952396	-2.357898
C	2.526223	2.952985	2.095351
C	2.975127	3.690133	0.965608
C	3.818367	4.804611	1.148582
H	4.231564	5.311871	0.267108
C	4.167800	5.223498	2.438629
H	4.822285	6.099441	2.561927
C	3.711598	4.516108	3.561068
H	3.988284	4.839496	4.575510
C	2.910573	3.380200	3.381678
H	2.554921	2.806578	4.250704
N	2.599908	3.271303	-0.336076
H	2.616985	2.261458	-0.537291
C	2.099053	4.029632	-1.368207
O	1.791339	3.528821	-2.452560
C	1.850054	5.504842	-1.148525
C	0.563357	5.947895	-0.739052
H	-0.200753	5.196526	-0.493871
C	0.265712	7.299158	-0.676027
H	-0.731876	7.639900	-0.359947
C	1.252206	8.263811	-1.023457
C	1.021411	9.666621	-0.949842
H	0.031733	10.030292	-0.631112
C	2.040131	10.548474	-1.269770
H	1.893175	11.637384	-1.219441
C	3.297557	10.016509	-1.667095
H	4.126045	10.703440	-1.919424
N	3.555611	8.721012	-1.760852
C	2.563226	7.835793	-1.455905
C	2.829931	6.424064	-1.532929
O	4.046793	5.905888	-1.860650
C	4.699263	6.324270	-3.065599
H	4.033801	6.153542	-3.939230
H	5.592399	5.678936	-3.161289
H	4.987674	7.390846	-3.013189
C	3.458703	-3.970281	2.882523

C	4.602989	-4.185940	2.057722
C	5.608016	-5.081819	2.492038
H	6.470560	-5.249281	1.837274
C	5.484709	-5.732472	3.725828
H	6.279462	-6.423834	4.045270
C	4.369848	-5.513972	4.549144
H	4.279016	-6.024434	5.519236
C	3.364784	-4.637426	4.117066
H	2.475982	-4.456732	4.740297
N	4.681032	-3.481389	0.848527
H	3.947480	-2.778397	0.658446
C	5.678702	-3.516559	-0.100925
O	6.645046	-4.282585	-0.064897
C	5.557651	-2.496136	-1.217905
C	6.665751	-2.473972	-2.118253
H	7.458164	-3.211852	-1.926442
C	6.731046	-1.589733	-3.175711
H	7.585924	-1.604878	-3.869300
C	5.698560	-0.627847	-3.367912
C	5.716451	0.338829	-4.412359
H	6.550244	0.335402	-5.132313
C	4.695057	1.269775	-4.495131
H	4.676111	2.033662	-5.286340
C	3.663314	1.245935	-3.515940
H	2.870806	2.014885	-3.519328
N	3.599526	0.349754	-2.538005
C	4.578902	-0.597932	-2.461471
C	4.504667	-1.588052	-1.416386
O	3.404365	-1.598157	-0.598495
C	2.182520	-2.061869	-1.210707
H	1.927208	-1.486121	-2.121188
H	1.390628	-1.922536	-0.453570
H	2.265945	-3.144797	-1.447970

Conformation 8.
Multiplicity: 2
Charge: 0
E(B97-3c) = -6287.348705406908 Hartree
E(M06/def2-TZVP) = -6287.343554937966 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -6285.165369469711 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -6285.340672448954 Hartree
E(PBEh-3c) = -6277.934632264553 Hartree
E(PM6) = 259.34585 Kcal/mol
E(PM7) = 116.68290 Kcal/mol
E(ωB97X-V/def2-TZVP) = -6289.236062146734 Hartree
E(GFN1-xTB) = -298.855723892688 Hartree
E(GFN2-xTB) = -290.686496946523 Hartree
E(GFN-FF) = -36.570043816992 Hartree

Coordinates:

Cu	-1.115358	-0.188219	1.239497
N	-1.474296	-1.895579	0.218181
N	-2.608213	0.728450	0.217924
N	-0.675700	1.556791	2.172303
N	0.312550	-1.119838	2.325356
C	-0.757526	-3.070906	0.302943
C	-1.236457	-4.018077	-0.683966
H	-0.829031	-5.024116	-0.829152
C	-2.274510	-3.408827	-1.343691
H	-2.895637	-3.810034	-2.151776
C	-2.424706	-2.088635	-0.760679
C	-3.441578	-1.180111	-1.127351
C	-3.511195	0.141488	-0.646388
C	-4.461927	1.132589	-1.115196
H	-5.310097	0.922741	-1.774859
C	-4.063057	2.338393	-0.596025
H	-4.513745	3.327042	-0.735993
C	-2.896769	2.076184	0.223949
C	-2.166476	3.079083	0.892324
C	-1.149603	2.808461	1.832176
C	-0.517374	3.817871	2.661663
H	-0.693664	4.895101	2.585285
C	0.289774	3.153476	3.548544
H	0.908941	3.574016	4.347873
C	0.216647	1.746191	3.210968
C	1.011076	0.750842	3.814571
C	1.047147	-0.587236	3.367486
C	1.934884	-1.597225	3.911454
H	2.633267	-1.435071	4.738435
C	1.732466	-2.740392	3.180059
H	2.224797	-3.712539	3.288434
C	0.722366	-2.430935	2.189561
C	0.262997	-3.351252	1.226770
C	-4.473851	-1.658218	-2.094792
C	-5.377093	-2.693949	-1.707872
C	-6.314683	-3.185641	-2.640438
H	-6.988390	-3.992416	-2.329133
C	-6.353787	-2.651921	-3.936101
H	-7.091210	-3.043501	-4.653289
C	-5.470167	-1.632522	-4.324746
H	-5.499980	-1.225809	-5.346367
C	-4.534166	-1.142185	-3.402043
H	-3.803668	-0.370931	-3.692541
N	-5.252622	-3.197760	-0.405676
H	-4.652819	-2.656713	0.231368
C	-5.508426	-4.485683	0.022124
O	-6.222152	-5.277795	-0.596493
C	-4.748547	-4.928461	1.259516
C	-4.818510	-6.328036	1.511903
H	-5.481149	-6.897426	0.843871
C	-4.092962	-6.938820	2.515872
H	-4.163537	-8.023919	2.684627
C	-3.209766	-6.163933	3.316476
C	-2.360734	-6.729337	4.311215
H	-2.419268	-7.811143	4.510045
C	-1.462180	-5.924596	4.991671
H	-0.783211	-6.338060	5.751784
C	-1.421436	-4.538386	4.676934
H	-0.689707	-3.878815	5.177697
N	-2.217294	-3.967948	3.786234
C	-3.111602	-4.738640	3.104638
C	-3.942906	-4.122097	2.095501
O	-3.941620	-2.787213	1.862908
C	-3.607343	-1.781956	2.828624
H	-4.043811	-2.025661	3.816579
H	-4.052005	-0.849258	2.432053
H	-2.512017	-1.682403	2.937333
C	-2.503660	4.507643	0.612621
C	-2.151052	5.121446	-0.628362
C	-2.412066	6.501168	-0.806052
H	-2.101953	6.970796	-1.745371
C	-3.039153	7.242141	0.202063
H	-3.234452	8.312268	0.033310
C	-3.418203	6.638197	1.409879
H	-3.918060	7.219414	2.198793
C	-3.141185	5.278935	1.603417
H	-3.416816	4.784719	2.547265
N	-1.581685	4.328664	-1.640882
H	-1.581171	3.307811	-1.502912
C	-1.082791	4.749520	-2.855677
O	-0.929773	5.938082	-3.158338
C	-0.756543	3.678100	-3.878095
C	-0.378099	4.192517	-5.154898
H	-0.327425	5.288397	-5.228765
C	-0.084169	3.377249	-6.229690
H	0.221445	3.803726	-7.197185
C	-0.226343	1.967341	-6.102143
C	-0.024998	1.061191	-7.181596
H	0.310866	1.454371	-8.154053
C	-0.272179	-0.289521	-7.000513
H	-0.133158	-1.013149	-7.817017
C	-0.735100	-0.727325	-5.729751
H	-0.979207	-1.792873	-5.567730
N	-0.902877	0.077988	-4.692429
C	-0.635910	1.405517	-4.839483
C	-0.821322	2.281309	-3.701595
O	-1.101725	1.786749	-2.474205
C	-0.440719	0.584855	-2.012330
H	-1.034612	-0.305242	-2.272618
H	-0.387455	0.693450	-0.916266
H	0.578803	0.511042	-2.437030
C	1.878896	1.103382	4.984036
C	3.067697	1.884706	4.854510
C	3.870761	2.110696	5.998792
H	4.784729	2.702310	5.877444
C	3.495537	1.590012	7.242763
H	4.135588	1.782081	8.117782
C	2.322380	0.833818	7.381642
H	2.024719	0.429110	8.360265
C	1.530929	0.595454	6.250597
H	0.610202	-0.001667	6.333440
N	3.382032	2.412512	3.594787
H	2.734988	2.202220	2.821670
C	4.387497	3.301961	3.270113
O	5.277647	3.642219	4.054956
C	4.329057	3.920051	1.886536
C	5.321766	4.916268	1.658067
H	6.031303	5.079494	2.481889
C	5.389959	5.637931	0.483798
H	6.166324	6.404041	0.335575
C	4.421262	5.420465	-0.533548
C	4.379038	6.185966	-1.733456
H	5.149428	6.954906	-1.903138
C	3.363523	5.973551	-2.649597
H	3.289577	6.559675	-3.577317
C	2.389611	4.979932	-2.360929
H	1.563948	4.806841	-3.070800
N	2.405092	4.230847	-1.268742
C	3.395020	4.420930	-0.350762
C	3.394709	3.637167	0.866700
O	2.484010	2.663208	1.107869
C	1.870513	1.874947	0.079239

H	0.998701	2.400744	-0.343623
H	1.560893	0.935751	0.575788
H	2.588280	1.661371	-0.731263
C	0.928283	-4.690032	1.189143
C	2.240611	-4.801890	0.646130
C	2.925974	-6.034752	0.718524
H	3.949463	-6.093443	0.329564
C	2.290924	-7.148801	1.284356
H	2.833177	-8.105492	1.331489
C	0.979363	-7.059334	1.776537
H	0.481587	-7.938789	2.211013
C	0.307747	-5.829247	1.727992
H	-0.710342	-5.734123	2.128407
N	2.770327	-3.658463	0.031287
H	2.096916	-2.915603	-0.206133
C	4.073503	-3.391125	-0.317861
O	5.021505	-4.147014	-0.097143
C	4.298596	-2.053067	-0.995682
C	5.646157	-1.583940	-0.973741
H	6.376799	-2.216314	-0.449332
C	6.013675	-0.396970	-1.575909
H	7.051465	-0.035581	-1.518867
C	5.048726	0.373293	-2.285533
C	5.343336	1.618384	-2.910725
H	6.364348	2.024989	-2.840411
C	4.345280	2.299647	-3.587634
H	4.535545	3.272292	-4.064145
C	3.047091	1.722371	-3.646623
H	2.235955	2.241975	-4.188384
N	2.726965	0.575728	-3.064707
C	3.691297	-0.099342	-2.373395
C	3.325716	-1.303662	-1.675302
O	2.001337	-1.665878	-1.623224
C	1.435077	-2.235191	-2.817888
H	1.446520	-1.494639	-3.641538
H	0.391788	-2.502968	-2.567304
H	1.994186	-3.150607	-3.108377

QUHVAS

Conformation 16.
Multiplicity: 4
Charge: 0
E(B97-3c) = -3413.539581620455 Hartree
E(M06/def2-TZVP) = -3413.225808808773 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3412.100375520925 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3412.314778635724 Hartree
E(PBEh-3c) = -3408.877130841416 Hartree
E(PM6) = 95.08553 Kcal/mol
E(PM7) = 109.71159 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3415.597894742145 Hartree
E(GFN1-xTB) = -148.541413151347 Hartree
E(GFN2-xTB) = -147.320508912646 Hartree
E(GFN-FF) = -20.504451894755 Hartree

Coordinates:

Co	-0.135033	0.030378	-0.336980
N	0.588906	-1.427145	0.766997
N	1.528759	0.658613	-1.025825
C	2.536625	-2.876839	1.670887
C	1.893502	-1.747278	0.789058
C	2.845146	-1.044804	0.002896
H	3.861765	-1.438206	0.074038
C	2.719056	0.067523	-0.861254
C	4.018328	0.457329	-1.636112
C	1.579016	-3.766697	2.486729
H	2.194663	-4.483149	3.068471
H	0.897053	-4.354052	1.847111
H	0.957000	-3.202667	3.202346
C	3.339372	-3.840727	0.760715
H	3.768705	-4.657273	1.376458
H	4.177696	-3.350321	0.230561
H	2.680413	-4.302771	-0.002167
C	3.489727	-2.186937	2.678096
H	3.987086	-2.948844	3.313441
H	2.926655	-1.502226	3.343865
H	4.276494	-1.592905	2.174752
C	3.913203	1.698521	-2.541515
H	4.869939	1.807966	-3.091743
H	3.748863	2.630319	-1.971223
H	3.105093	1.620360	-3.291069
C	4.381760	-0.743355	-2.545150
H	5.303968	-0.518687	-3.120183
H	3.567736	-0.947956	-3.270035
H	4.554814	-1.670294	-1.965698
C	5.168732	0.720678	-0.635820
H	6.088108	1.003897	-1.188082
H	5.411148	-0.163591	-0.016077
H	4.914027	1.555098	0.048410
C	-0.472080	-2.105129	1.427102
C	-1.092907	-3.214314	0.783151
C	-2.183131	-3.832719	1.418722
H	-2.665277	-4.698942	0.940785
C	-2.674618	-3.359422	2.643971
H	-3.532834	-3.853815	3.123322
C	-2.078672	-2.243039	3.243743
H	-2.476937	-1.864038	4.197997
C	-0.975833	-1.597765	2.656057
C	-0.613132	-3.678816	-0.587723
H	0.438447	-3.343113	-0.697071
C	-0.625362	-5.202756	-0.763506
H	-0.051469	-5.711087	0.038114
H	-0.173847	-5.481907	-1.737306
H	-1.655244	-5.615730	-0.754432
C	-1.424791	-2.980018	-1.695381
H	-1.424387	-1.879253	-1.552275
H	-2.485913	-3.303907	-1.673070
H	-1.012546	-3.207702	-2.700471
C	-0.336040	-0.394138	3.339617
H	0.525045	-0.085790	2.711777
C	0.204931	-0.744657	4.736665
H	0.921386	-1.589939	4.704334
H	-0.614092	-1.029566	5.429401
H	0.727184	0.127277	5.181858
C	-1.301606	0.800334	3.408217
H	-1.641727	1.092919	2.398229
H	-0.806957	1.678021	3.872733
H	-2.200137	0.561071	4.014516
C	1.174559	1.876320	-1.651735
C	0.390023	1.838635	-2.843087
C	-0.022344	3.057228	-3.411869
H	-0.618200	3.043825	-4.337474
C	0.314093	4.283293	-2.824751
H	-0.007865	5.226254	-3.291348
C	1.041830	4.304319	-1.624104
H	1.275612	5.269853	-1.151860
C	1.465153	3.118241	-1.005481
C	0.012649	0.513546	-3.497332
H	0.310699	-0.294118	-2.789282
C	-1.502568	0.385515	-3.721623
H	-2.056482	0.495518	-2.768256
H	-1.747881	-0.610454	-4.143190
H	-1.878955	1.150379	-4.431337
C	0.797339	0.281416	-4.799678
H	1.892094	0.322485	-4.631543
H	0.545428	1.053379	-5.556394
H	0.554114	-0.710172	-5.233486
C	2.142590	3.121774	0.359763
H	2.824451	2.247832	0.392045
C	1.086748	2.904244	1.461021
H	1.565106	2.755085	2.450708
H	0.458676	2.015674	1.242523
H	0.400275	3.772277	1.528369
C	2.987664	4.369369	0.637582
H	3.736366	4.546598	-0.161547
H	3.531408	4.256473	1.597171
H	2.363195	5.282232	0.726908
N	-1.865150	0.354268	-0.066474
C	-2.996932	0.945529	0.053072
C	-3.065739	2.401774	0.404656
C	-2.148878	3.302895	-0.176154
H	-1.435010	2.931818	-0.925655
C	-2.152949	4.655305	0.189303
H	-1.439089	5.344225	-0.287166
C	-3.059695	5.124722	1.154322
H	-3.058291	6.186233	1.445935
C	-3.971107	4.233247	1.744368
H	-4.678956	4.592638	2.507192
C	-3.982537	2.883281	1.365476
H	-4.694742	2.184780	1.830251
C	-4.269168	0.181803	-0.138137
C	-4.273260	-1.209661	0.102714
H	-3.349446	-1.682231	0.462453
C	-5.434321	-1.963296	-0.099580
H	-5.422650	-3.044497	0.109482
C	-6.610122	-1.342518	-0.557540
H	-7.523914	-1.935217	-0.717817
C	-6.614569	0.039623	-0.806285
H	-7.529740	0.530986	-1.171216
C	-5.454829	0.799839	-0.593411
H	-5.460469	1.881413	-0.795476

Conformation 20.
Multiplicity: 4
Charge: 0
E(B97-3c) = -3413.537101997373 Hartree
E(M06/def2-TZVP) = -3413.222595181089 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3412.098679869604 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3412.312788690261 Hartree
E(PBEh-3c) = -3408.871848368477 Hartree
E(PM6) = 98.56898 Kcal/mol

E(PM7) = 113.04935 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3415.593775659198 Hartree
E(GFN1-xTB) = -148.535663096653 Hartree
E(GFN2-xTB) = -147.314873545114 Hartree
E(GFN-FF) = -20.502125605986 Hartree

Coordinates:

Co	0.253011	0.121641	0.146248
N	-1.268137	-0.929560	0.802848
N	-0.498980	1.854874	0.427515
C	-3.580710	-1.203577	1.877144
C	-2.366018	-0.360834	1.350113
C	-2.474818	1.043648	1.496874
H	-3.371210	1.377552	2.017197
C	-1.622590	2.107823	1.104780
C	-2.063337	3.522817	1.599858
C	-4.766794	-0.320806	2.324850
H	-5.602621	-0.982563	2.628080
H	-5.136365	0.331473	1.509114
H	-4.521986	0.311832	3.200949
C	-4.121367	-2.134451	0.772672
H	-5.038527	-2.640640	1.136870
H	-3.394222	-2.918557	0.503331
H	-4.386082	-1.567175	-0.141477
C	-3.171022	-2.055156	3.098888
H	-4.067939	-2.560799	3.512258
H	-2.734703	-1.427423	3.901217
H	-2.441672	-2.838401	2.827969
C	-2.017505	3.491765	3.149010
H	-2.314922	4.480260	3.556042
H	-0.992490	3.267469	3.507378
H	-2.695762	2.726463	3.572272
C	-3.506987	3.823750	1.134201
H	-3.812565	4.829400	1.488753
H	-4.243628	3.094802	1.522520
H	-3.578778	3.820162	0.027690
C	-1.177651	4.696278	1.142152
H	-1.544620	5.620658	1.632912
H	-1.214220	4.861131	0.050599
H	-0.116899	4.568100	1.423894
C	-0.950632	-2.317055	0.731702
C	-1.185574	-3.047514	-0.471992
C	-0.765572	-4.388774	-0.535241
H	-0.945214	-4.960755	-1.458204
C	-0.124636	-5.009059	0.543639
H	0.187082	-6.061969	0.473195
C	0.141613	-4.269531	1.703114
H	0.677571	-4.745887	2.537846
C	-0.238230	-2.919985	1.814734
C	-1.835962	-2.404319	-1.696029
H	-2.286389	-1.447318	-1.361885
C	-0.785134	-2.062087	-2.767004
H	-0.027595	-1.360431	-2.374972
H	-1.266368	-1.597100	-3.651940
H	-0.253372	-2.974663	-3.108149
C	-2.946847	-3.271729	-2.312213
H	-3.700444	-3.586456	-1.565009
H	-2.532749	-4.189197	-2.779019
H	-3.470872	-2.711336	-3.113333
C	0.195856	-2.103829	3.032011
H	-0.456164	-1.208641	3.080084
C	1.641377	-1.600230	2.849837
H	1.765997	-1.078180	1.879567
H	2.360874	-2.444825	2.853767
H	1.922201	-0.904253	3.667825
C	0.061236	-2.856035	4.363651
H	-0.958341	-3.261678	4.514771
H	0.289775	-2.177911	5.211087
H	0.774446	-3.703537	4.430162
C	0.382821	2.711731	-0.270783
C	1.726335	2.847690	0.193365
C	2.615123	3.641838	-0.553014
H	3.649863	3.766075	-0.200072
C	2.208638	4.271730	-1.735187
H	2.916601	4.895640	-2.300737
C	0.902741	4.079475	-2.213089
H	0.601735	4.548562	-3.161000
C	-0.023232	3.289236	-1.514672
C	2.190886	2.159916	1.473472
H	1.425341	1.382437	1.717176
C	3.533220	1.435289	1.305170
H	3.491583	0.707795	0.471337
H	3.787060	0.877529	2.229057
H	4.363221	2.144395	1.108847
C	2.219897	3.132545	2.664265
H	1.230182	3.599034	2.837668
H	2.948597	3.950594	2.485343
H	2.518638	2.607487	3.594724
C	-1.401735	2.976037	-2.085651
H	-2.107175	2.908513	-1.232474
C	-1.387016	1.589109	-2.756574
H	-2.408803	1.281427	-3.059369
H	-0.987159	0.819017	-2.066742
H	-0.738643	1.587286	-3.656174
C	-1.943771	4.047712	-3.036963
H	-1.939030	5.054227	-2.570722
H	-2.986998	3.809115	-3.326314
H	-1.354129	4.104081	-3.975206
N	1.529363	-0.817697	-0.671093
C	2.475184	-1.164911	-1.464857
C	2.583257	-0.585400	-2.842748
C	2.236210	0.764810	-3.062297
H	1.952055	1.388954	-2.204047
C	2.264731	1.306785	-4.353233
H	2.006958	2.367002	-4.499172
C	2.624286	0.504466	-5.449234
H	2.641606	0.928916	-6.464803
C	2.966120	-0.842263	-5.242528
H	3.241988	-1.478673	-6.097487
C	2.956188	-1.382049	-3.948365
H	3.219660	-2.438418	-3.788559
C	3.477651	-2.184664	-1.022440
C	3.075253	-3.190029	-0.116639
H	2.023801	-3.222183	0.200180
C	3.997010	-4.129971	0.357760
H	3.661947	-4.916145	1.052412
C	5.339822	-4.074849	-0.055482
H	6.066100	-4.812427	0.319276
C	5.750661	-3.075814	-0.953071
H	6.801931	-3.023525	-1.275985
C	4.825973	-2.139906	-1.440242
H	5.151640	-1.355200	-2.139754

Conformation 21.
Multiplicity: 4
Charge: 0
E(B97-3c) = -3413.535794721675 Hartree
E(M06/def2-TZVP) = -3413.221368215538 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3412.097389635454 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3412.312508426199 Hartree
E(PBEh-3c) = -3408.871439088500 Hartree
E(PM6) = 99.56668 Kcal/mol
E(PM7) = 107.19404 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3415.592108477200 Hartree
E(GFN1-xTB) = -148.533934476783 Hartree
E(GFN2-xTB) = -147.311344835929 Hartree
E(GFN-FF) = -20.493475506248 Hartree

Coordinates:

Co	-0.063504	-0.442176	0.430065
N	0.872075	-0.398027	-1.320972
N	-1.825498	-0.841831	-0.236113
C	0.925921	-0.779436	-3.892851
C	0.251307	-0.707443	-2.471938
C	-1.127114	-1.052104	-2.510432
H	-1.488826	-1.310049	-3.507905
C	-2.132898	-1.088898	-1.518809
C	-3.559504	-1.456684	-2.054362
C	0.850098	-2.252828	-4.367878
H	1.319099	-2.349205	-5.368935
H	-0.189485	-2.625137	-4.442445
H	1.397801	-2.918624	-3.670815
C	0.136074	0.126511	-4.871290
H	0.609731	0.092348	-5.873766
H	0.143586	1.180175	-4.527264
H	-0.920393	-0.178490	-4.991638
C	2.403299	-0.355297	-4.014322
H	2.691351	-0.445030	-5.082008
H	3.087480	-0.993359	-3.430471
H	2.580887	0.689560	-3.707011
C	-3.483844	-2.830293	-2.768292
H	-4.486400	-3.100319	-3.158956
H	-3.168364	-3.629158	-2.068823
H	-2.780430	-2.832257	-3.622299
C	-4.005523	-0.386553	-3.080369
H	-5.010743	-0.642350	-3.474212
H	-3.312056	-0.312277	-3.940362
H	-4.071363	0.616010	-2.613666
C	-4.666641	-1.569129	-0.989358
H	-5.591994	-1.925608	-1.486087
H	-4.897407	-0.603432	-0.507335
H	-4.415952	-2.289286	-0.190849
C	2.231105	0.002874	-1.196519
C	2.561940	1.387077	-1.224579
C	3.915307	1.754828	-1.113976
H	4.185599	2.821738	-1.151757
C	4.923826	0.795751	-0.958177
H	5.977196	1.105568	-0.885873
C	4.575664	-0.557582	-0.856161
H	5.362025	-1.309703	-0.687964
C	3.236355	-0.974991	-0.953100
C	1.492960	2.465773	-1.368321

H	0.510693	1.951461	-1.389307
C	1.491377	3.413728	-0.157450
H	1.329572	2.856563	0.783237
H	0.683932	4.168350	-0.250631
H	2.452450	3.961894	-0.070471
C	1.635820	3.260325	-2.677852
H	1.597568	2.603241	-3.568905
H	2.599217	3.810739	-2.711085
H	0.821245	4.007837	-2.771725
C	2.877229	-2.441587	-0.747007
H	1.811012	-2.559182	-1.031511
C	3.009019	-2.800029	0.745079
H	2.428847	-2.094373	1.371206
H	4.067567	-2.738583	1.072507
H	2.651221	-3.832262	0.941091
C	3.699674	-3.398970	-1.623008
H	3.616040	-3.147504	-2.699457
H	3.353439	-4.444286	-1.488343
H	4.776534	-3.373962	-1.356675
C	-2.667336	-0.649497	0.884605
C	-3.374942	0.585591	1.030532
C	-4.179825	0.770718	2.164491
H	-4.741908	1.709630	2.275490
C	-4.267188	-0.208228	3.164285
H	-4.905717	-0.047503	4.045909
C	-3.514527	-1.383151	3.044446
H	-3.555570	-2.142920	3.841369
C	-2.701588	-1.630837	1.922071
C	-3.195866	1.698269	0.004683
H	-2.912894	1.220199	-0.953676
C	-4.466095	2.518520	-0.250010
H	-5.326850	1.872360	-0.518215
H	-4.301128	3.231545	-1.083077
H	-4.757107	3.119848	0.635905
C	-2.015465	2.600921	0.408166
H	-1.103161	1.999361	0.598692
H	-2.231970	3.159436	1.341501
H	-1.785241	3.331404	-0.394202
C	-1.910808	-2.938968	1.883723
H	-2.092612	-3.408790	2.874534
C	-0.389079	-2.755174	1.781732
H	0.139928	-3.708381	1.987858
H	-0.001533	-2.003041	2.496205
H	-0.069976	-2.487707	0.740530
C	-2.405669	-3.934592	0.822304
H	-3.493880	-4.121552	0.913328
H	-1.882862	-4.906918	0.932519
H	-2.200752	-3.559094	-0.198734
N	0.963398	0.318806	1.684879
C	1.299950	1.015162	2.707392
C	2.683802	0.921285	3.271110
C	3.740403	0.504254	2.433004
H	3.520155	0.293007	1.378838
C	5.040210	0.376356	2.933585
H	5.851486	0.064130	2.257522
C	5.308400	0.654658	4.285477
H	6.331033	0.554512	4.680708
C	4.263875	1.066251	5.129431
H	4.464443	1.281275	6.190454
C	2.961288	1.204362	4.627064
H	2.146233	1.523788	5.293656
C	0.332226	1.962802	3.357386
C	0.711760	3.293065	3.644309
H	1.740060	3.619087	3.425659
C	-0.212444	4.196799	4.186614
H	0.092068	5.235448	4.388131
C	-1.520715	3.776364	4.478979
H	-2.242448	4.481192	4.919595
C	-1.901575	2.452112	4.208659
H	-2.921569	2.109498	4.435812
C	-0.987854	1.555282	3.637385
H	-1.297769	0.524995	3.405889

Conformation 24.
Multiplicity: 4
Charge: 0
E(B97-3c) = -3413.522213598330 Hartree
E(M06/def2-TZVP) = -3413.209283793482 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3412.084606376122 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3412.298501840146 Hartree
E(PBEh-3c) = -3408.856680718656 Hartree
E(PM6) = 105.36936 Kcal/mol
E(PM7) = 118.40729 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3415.576821403597 Hartree
E(GFN1-xTB) = -148.524828018604 Hartree
E(GFN2-xTB) = -147.299872495061 Hartree
E(GFN-FF) = -20.494233203666 Hartree

Coordinates:

Co	-0.091171	0.500574	-0.303213
N	-1.150774	-1.153966	-0.547752
N	1.588373	-0.130306	-0.977502
C	-1.340369	-3.660095	-1.175660
C	-0.629804	-2.258548	-1.098287
C	0.700031	-2.271449	-1.606204
H	0.970918	-3.202185	-2.107764
C	1.741778	-1.316941	-1.592437
C	2.994293	-1.708320	-2.441373
C	-2.855688	-3.667729	-0.898945
H	-3.221392	-4.709991	-0.999778
H	-3.416661	-3.040999	-1.615182
H	-3.111439	-3.320703	0.114571
C	-1.150317	-4.329366	-2.560380
H	-1.689212	-5.298374	-2.564365
H	-0.093443	-4.551844	-2.800837
H	-1.567085	-3.711434	-3.378262
C	-0.645475	-4.552942	-0.116212
H	-1.119705	-5.556277	-0.095332
H	-0.727683	-4.114501	0.896810
H	0.431969	-4.682149	-0.337802
C	2.517105	-1.784229	-3.915079
H	3.367190	-2.054698	-4.575355
H	2.124616	-0.801905	-4.248888
H	1.715260	-2.533738	-4.058217
C	3.541171	-3.085883	-2.003426
H	4.440991	-3.339981	-2.600609
H	2.808621	-3.903185	-2.146852
H	3.833435	-3.077381	-0.935603
C	4.163734	-0.708170	-2.407992
H	4.942375	-1.060705	-3.114769
H	4.630705	-0.619022	-1.411820
H	3.860310	0.305673	-2.724922
C	-2.507503	-0.898884	-0.214623
C	-3.351022	-0.343620	-1.231321
C	-4.701500	-0.094210	-0.929416
H	-5.351835	0.309024	-1.722468
C	-5.218469	-0.308832	0.353697
H	-6.274655	-0.096462	0.575765
C	-4.351340	-0.732095	1.362418
H	-4.730021	-0.831710	2.392383
C	-2.992741	-1.026011	1.120686
C	-2.870729	0.070987	-2.626576
H	-3.738427	0.616832	-3.055920
C	-1.715174	1.084395	-2.606173
H	-1.883308	1.884546	-1.860174
H	-1.587949	1.558538	-3.601403
H	-0.744341	0.578012	-2.391149
C	-2.566281	-1.079003	-3.598451
H	-3.392908	-1.816149	-3.631744
H	-1.634026	-1.607370	-3.321602
H	-2.426288	-0.681519	-4.625179
C	-2.206069	-1.467667	2.365141
H	-2.544933	-0.753498	3.149427
C	-0.678489	-1.361991	2.353825
H	-0.344409	-0.351518	2.049042
H	-0.195251	-2.099554	1.685321
H	-0.296769	-1.542326	3.379197
C	-2.641978	-2.867552	2.846859
H	-3.742888	-2.948506	2.941240
H	-2.194924	-3.091172	3.837305
H	-2.309777	-3.658525	2.146067
C	2.579195	0.780785	-0.523922
C	3.401628	0.447805	0.597720
C	4.301162	1.413905	1.080545
H	4.942712	1.160514	1.938892
C	4.388479	2.690337	0.510545
H	5.096225	3.431428	0.911410
C	3.559356	3.016002	-0.570117
H	3.620745	4.019857	-1.018454
C	2.656704	2.082016	-1.107045
C	3.301768	-0.895303	1.314405
H	2.595041	-1.531088	0.744274
C	4.652060	-1.630006	1.379385
H	5.110603	-1.751187	0.378354
H	4.524913	-2.639361	1.821770
H	5.379369	-1.082541	2.013918
C	2.723112	-0.716587	2.728993
H	1.775690	-0.148139	2.712223
H	3.425899	-0.158458	3.381490
H	2.530962	-1.701847	3.201181
C	1.786209	2.474450	-2.294344
H	1.227581	1.565673	-2.599729
C	2.620507	2.922995	-3.505675
H	1.963022	3.139144	-4.372656
H	3.344919	2.142197	-3.813182
H	3.195936	3.846325	-3.287332
C	0.759419	3.549495	-1.896455
H	0.134785	3.213011	-1.043477
H	0.083791	3.787468	-2.743450
H	1.263269	4.489796	-1.590601
N	-0.976419	1.630651	0.760727
C	-1.217696	2.369947	1.779776

C	-2.488557	3.152291	1.870471
C	-3.574556	2.793098	1.040231
H	-3.458808	1.926680	0.374399
C	-4.771895	3.514096	1.080873
H	-5.611278	3.207243	0.437581
C	-4.906338	4.615754	1.944873
H	-5.849028	5.183375	1.977716
C	-3.830592	4.987559	2.766979
H	-3.925019	5.853837	3.439890
C	-2.630662	4.261240	2.734128
H	-1.789150	4.563934	3.374681
C	-0.226177	2.443533	2.904665
C	1.140574	2.651760	2.622366
H	1.460247	2.798492	1.579737
C	2.083168	2.678679	3.659367
H	3.141808	2.857355	3.419395
C	1.680085	2.467596	4.987800
H	2.422551	2.480057	5.800381
C	0.324432	2.237347	5.275911
H	0.003505	2.059174	6.313920
C	-0.625052	2.238207	4.243882
H	-1.688856	2.066022	4.468850

Conformation 25.
Multiplicity: 4
Charge: 0
E(B97-3c) = -3413.534120938863 Hartree
E(M06/def2-TZVP) = -3413.218951084109 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3412.095580918157 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3412.309826816540 Hartree
E(PBEh-3c) = -3408.866317617005 Hartree
E(PM6) = 101.74523 Kcal/mol
E(PM7) = 113.44669 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3415.587721198738 Hartree
E(GFN1-xTB) = -148.531934483411 Hartree
E(GFN2-xTB) = -147.310010848297 Hartree
E(GFN-FF) = -20.495824033238 Hartree

Coordinates:

Co	0.217598	-0.409987	-0.096342
N	0.128325	0.292893	1.748532
N	-1.562905	-1.110090	-0.192172
C	-1.163725	0.845506	3.920626
C	-0.960562	0.166169	2.518386
C	-2.101575	-0.568137	2.079826
H	-2.879533	-0.657650	2.835042
C	-2.421254	-1.173799	0.848536
C	-3.767831	-1.964179	0.758084
C	-2.115902	2.044260	3.676920
H	-2.305259	2.579150	4.630908
H	-3.089496	1.712375	3.265852
H	-1.676098	2.767110	2.963291
C	-1.838259	-0.120667	4.928434
H	-1.884485	0.370806	5.920911
H	-1.260476	-1.058253	5.042337
H	-2.877280	-0.388442	4.658176
C	0.102445	1.372558	4.624275
H	-0.199990	1.801248	5.601620
H	0.618635	2.164995	4.060019
H	0.840581	0.574411	4.822507
C	-3.503850	-3.358946	0.152230
H	-4.433855	-3.962323	0.185287
H	-2.722985	-3.904065	0.719776
H	-3.188035	-3.295340	-0.903853
C	-4.819783	-1.228251	-0.102174
H	-5.775483	-1.791605	-0.072954
H	-4.514038	-1.146643	-1.160657
H	-5.016740	-0.209968	0.288106
C	-4.401452	-2.189812	2.148018
H	-5.295420	-2.834469	2.030865
H	-4.743648	-1.246221	2.617564
H	-3.706838	-2.697055	2.846266
C	1.401433	0.792191	2.133857
C	2.378174	-0.122331	2.629154
C	3.635451	0.387952	3.005269
H	4.384658	-0.311486	3.410241
C	3.960849	1.741279	2.848459
H	4.952712	2.113148	3.145585
C	3.023511	2.604258	2.268804
H	3.290593	3.659364	2.101724
C	1.743471	2.155581	1.898555
C	2.173679	-1.636523	2.726200
H	3.168811	-2.025495	3.033394
C	1.178451	-2.103589	3.800164
H	1.399875	-1.651154	4.787379
H	1.233946	-3.205980	3.915428
H	0.135136	-1.853859	3.526300
C	1.873076	-2.304640	1.373497
H	2.551614	-1.944995	0.577346
H	0.814107	-2.132366	1.057992
H	1.976586	-3.406943	1.450823
C	0.762221	3.130183	1.255960
H	-0.198368	2.589222	1.130966
C	1.235472	3.551294	-0.146338
H	1.353903	2.673495	-0.805734
H	2.212754	4.075211	-0.098628
H	0.504936	4.240488	-0.617463
C	0.505359	4.370883	2.128986
H	0.183038	4.103862	3.154648
H	-0.284558	5.005502	1.677296
H	1.417518	4.996380	2.218746
C	-1.852661	-1.271812	-1.572939
C	-2.537503	-0.217749	-2.261344
C	-2.789287	-0.366164	-3.634618
H	-3.329069	0.428682	-4.169731
C	-2.340941	-1.490939	-4.342592
H	-2.547233	-1.586039	-5.419367
C	-1.606200	-2.478510	-3.676592
H	-1.224623	-3.343088	-4.240752
C	-1.347751	-2.394326	-2.295801
C	-2.880778	1.082488	-1.538663
H	-3.057408	0.839750	-0.472562
C	-1.674241	2.037878	-1.581936
H	-0.742692	1.540991	-1.235780
H	-1.845778	2.923370	-0.936694
H	-1.475935	2.387262	-2.615358
C	-4.139534	1.779410	-2.068563
H	-5.016223	1.101335	-2.076207
H	-3.996454	2.162721	-3.099948
H	-4.388519	2.653808	-1.433796
C	-0.490891	-3.457137	-1.616727
H	-0.600249	-3.309360	-0.522140
C	0.993083	-3.251305	-1.975075
H	1.635902	-3.986385	-1.448560
H	1.341617	-2.235121	-1.699714
H	1.155902	-3.372205	-3.066066
C	-0.933220	-4.892329	-1.940805
H	-2.002661	-5.056782	-1.704123
H	-0.336251	-5.620390	-1.354531
H	-0.782301	-5.136722	-3.012534
N	1.657645	0.166187	-0.981753
C	2.429732	0.556065	-1.928886
C	3.912601	0.407434	-1.793974
C	4.481359	0.344634	-0.502261
H	3.820491	0.452837	0.368439
C	5.858787	0.162949	-0.338421
H	6.283633	0.130611	0.677056
C	6.694018	0.031664	-1.461960
H	7.778002	-0.111707	-1.333928
C	6.138019	0.087521	-2.750400
H	6.784710	-0.021407	-3.634783
C	4.758373	0.278461	-2.918046
H	4.326950	0.313401	-3.929537
C	1.871371	1.178391	-3.173541
C	0.716271	0.636489	-3.775505
H	0.259384	-0.268887	-3.349079
C	0.156419	1.242145	-4.908515
H	-0.735148	0.795593	-5.372944
C	0.726025	2.409749	-5.442357
H	0.281408	2.887294	-6.328997
C	1.867431	2.965189	-4.840723
H	2.313968	3.885631	-5.247590
C	2.443341	2.348446	-3.721280
H	3.337873	2.783464	-3.250346

Conformation 26.
Multiplicity: 4
Charge: 0
E(B97-3c) = -3413.527433727270 Hartree
E(M06/def2-TZVP) = -3413.214203684880 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3412.089406301248 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3412.304146377179 Hartree
E(PBEh-3c) = -3408.864841198544 Hartree
E(PM6) = 101.41495 Kcal/mol
E(PM7) = 116.72492 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3415.587044619962 Hartree
E(GFN1-xTB) = -148.527441701144 Hartree
E(GFN2-xTB) = -147.305221332721 Hartree
E(GFN-FF) = -20.492337919882 Hartree

Coordinates:

Co	0.099354	-0.336096	-0.050237
N	-1.675722	-1.037815	0.075784
N	-0.106581	1.168039	1.217054
C	-3.981119	-1.348982	1.124036
C	-2.613951	-0.612522	0.943738
C	-2.378130	0.528152	1.740116
H	-3.216457	0.810051	2.374760
C	-1.251610	1.391199	1.876049
C	-1.524847	2.592288	2.853450
C	-4.860923	-0.705079	2.216482
H	-5.801116	-1.285411	2.302953

H	-5.141739	0.338993	1.973891
H	-4.370936	-0.716070	3.210101
C	-4.794379	-1.322083	-0.185701
H	-5.779428	-1.806335	-0.024482
H	-4.286180	-1.861645	-1.004025
H	-4.979742	-0.279540	-0.512930
C	-3.743569	-2.814955	1.547295
H	-4.715864	-3.292778	1.784733
H	-3.106614	-2.875706	2.452394
H	-3.271885	-3.408754	0.744378
C	-1.947816	2.029868	4.234091
H	-2.109786	2.868970	4.941165
H	-1.154483	1.380314	4.656000
H	-2.883696	1.441018	4.198161
C	-2.678910	3.428809	2.246161
H	-2.904308	4.293207	2.904088
H	-3.608393	2.841564	2.122468
H	-2.393200	3.823037	1.249991
C	-0.365962	3.570864	3.125898
H	-0.749163	4.366066	3.797583
H	0.014246	4.059903	2.213806
H	0.493781	3.095453	3.628930
C	-1.729035	-2.070544	-0.898051
C	-1.208636	-3.362363	-0.543477
C	-1.219392	-4.391609	-1.495370
H	-0.831200	-5.383441	-1.220448
C	-1.703376	-4.171365	-2.791243
H	-1.714409	-4.989226	-3.526802
C	-2.124275	-2.889840	-3.153806
H	-2.442637	-2.706601	-4.192494
C	-2.125774	-1.804443	-2.250222
C	-0.534034	-3.588286	0.806992
H	-0.892138	-2.798576	1.497690
C	-0.846151	-4.947438	1.447047
H	-1.935610	-5.119624	1.550384
H	-0.392617	-5.005554	2.457183
H	-0.424937	-5.787540	0.857647
C	0.987347	-3.405771	0.648712
H	1.238404	-2.422364	0.192432
H	1.413450	-4.181301	-0.020818
H	1.504788	-3.466381	1.626861
C	-2.456553	-0.438309	-2.883957
H	-1.775202	-0.404889	-3.764235
C	-2.143733	0.833422	-2.088836
H	-1.080121	0.863119	-1.774736
H	-2.775074	0.951712	-1.187832
H	-2.309139	1.716239	-2.739986
C	-3.885300	-0.368296	-3.461327
H	-4.136223	-1.261799	-4.065986
H	-3.982979	0.520220	-4.117699
H	-4.646070	-0.279764	-2.663351
C	1.103315	1.904593	1.351502
C	2.041949	1.525137	2.351407
C	3.251972	2.236177	2.442503
H	3.978147	1.960272	3.222777
C	3.554125	3.275511	1.553235
H	4.508834	3.816011	1.635410
C	2.642039	3.603312	0.541789
H	2.887905	4.405858	-0.170708
C	1.410296	2.936227	0.420599
C	1.785442	0.338615	3.274414
H	0.733887	0.021420	3.121021
C	2.685695	-0.842205	2.867847
H	2.549949	-1.087707	1.796626
H	2.455621	-1.744608	3.472010
H	3.757829	-0.597409	3.018336
C	1.952181	0.680815	4.762548
H	1.292703	1.517711	5.068048
H	2.995269	0.971707	5.003725
H	1.702995	-0.196896	5.393405
C	0.431422	3.337282	-0.678830
H	-0.492358	2.744835	-0.519878
C	0.969522	2.980344	-2.075299
H	0.235099	3.257272	-2.859739
H	1.169952	1.896156	-2.159955
H	1.916039	3.517840	-2.294085
C	0.049199	4.825262	-0.604537
H	-0.364517	5.096941	0.386927
H	-0.714228	5.068948	-1.371429
H	0.924564	5.481367	-0.789642
N	1.663811	-0.268577	-0.903759
C	2.561028	-0.407077	-1.809405
C	4.007046	-0.484644	-1.434022
C	4.929625	-1.249483	-2.181557
H	4.587483	-1.783512	-3.080854
C	6.267276	-1.346974	-1.770957
H	6.974023	-1.955895	-2.355782
C	6.704031	-0.672083	-0.619081
H	7.756539	-0.742408	-0.304248
C	5.791525	0.095285	0.126282
H	6.125184	0.636609	1.025424
C	4.453454	0.183741	-0.273820
H	3.730801	0.780163	0.299155
C	2.190175	-0.478081	-3.260607
C	1.049766	-1.206368	-3.659609
H	0.478756	-1.763939	-2.902491
C	0.658948	-1.234410	-5.005160
H	-0.219513	-1.827601	-5.303000
C	1.388260	-0.517767	-5.969040
H	1.076385	-0.533067	-7.024447
C	2.522277	0.214472	-5.580470
H	3.097508	0.780467	-6.329620
C	2.927986	0.225822	-4.238298
H	3.818065	0.797175	-3.933911

Conformation 27.
Multiplicity: 4
Charge: 0
E(B97-3c) = -3413.527900609814 Hartree
E(M06/def2-TZVP) = -3413.218268966413 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3412.089538559284 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3412.305313805650 Hartree
E(PBEh-3c) = -3408.861985515107 Hartree
E(PM6) = 104.83845 Kcal/mol
E(PM7) = 111.70127 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3415.582289098760 Hartree
E(GFN1-xTB) = -148.527088177185 Hartree
E(GFN2-xTB) = -147.303018689219 Hartree
E(GFN-FF) = -20.492925981894 Hartree

Coordinates:

Co	0.315487	-0.117045	-0.137706
N	-0.479683	1.076984	1.265000
N	-0.475661	0.709218	-1.690937
C	-1.577513	3.331105	1.904620
C	-1.203505	2.155317	0.922368
C	-1.580603	2.414000	-0.424099
H	-2.205619	3.298155	-0.537148
C	-1.288760	1.775593	-1.652881
C	-2.027229	2.383957	-2.894328
C	-2.979384	3.918549	1.599386
H	-3.230074	4.669832	2.374663
H	-3.765158	3.138212	1.619335
H	-3.038377	4.440884	0.625471
C	-1.571040	3.016691	3.415005
H	-1.888661	3.931603	3.955859
H	-0.577906	2.734793	3.799255
H	-2.273728	2.207859	3.682319
C	-0.518755	4.433343	1.644190
H	-0.713742	5.310535	2.295960
H	-0.537337	4.770351	0.589109
H	0.502064	4.066589	1.866364
C	-1.933771	3.930459	-2.892789
H	-2.429981	4.324885	-3.802555
H	-0.879704	4.270204	-2.907235
H	-2.433490	4.400628	-2.024964
C	-3.515683	1.973663	-2.770972
H	-4.096472	2.385839	-3.622345
H	-3.963431	2.347637	-1.829513
H	-3.627104	0.871641	-2.784572
C	-1.513917	1.925347	-4.273238
H	-2.069599	2.482716	-5.054555
H	-1.672863	0.850482	-4.458256
H	-0.437452	2.132672	-4.413125
C	-0.281077	0.593508	2.586459
C	0.918006	0.895602	3.294570
C	1.067591	0.428099	4.612021
H	1.984599	0.675187	5.168590
C	0.079104	-0.350801	5.224089
H	0.204141	-0.699826	6.260176
C	-1.052567	-0.716739	4.485466
H	-1.811766	-1.373812	4.939448
C	-1.253420	-0.278692	3.161843
C	2.043587	1.696277	2.653142
H	1.643926	2.116378	1.706876
C	2.519785	2.870836	3.522909
H	1.683891	3.535072	3.820799
H	3.264439	3.483303	2.974047
H	3.011663	2.516054	4.451890
C	3.217417	0.766006	2.296109
H	2.877159	-0.061591	1.644757
H	3.651917	0.311422	3.210122
H	4.023042	1.326376	1.777690
C	-2.500587	-0.796448	2.438892
H	-2.900274	-1.580774	3.117882
C	-2.211538	-1.500981	1.105768
H	-1.394623	-2.241012	1.198313
H	-1.938164	-0.774170	0.310454
H	-3.118566	-2.030533	0.748703
C	-3.626335	0.237734	2.269736
H	-3.884178	0.728380	3.229397
H	-4.542559	-0.258897	1.888162

H	-3.348218	1.020471	1.537665
C	0.093348	0.037725	-2.802129
C	-0.585155	-1.067266	-3.400963
C	0.007402	-1.708661	-4.500362
H	-0.517172	-2.551328	-4.975686
C	1.254336	-1.306599	-4.994497
H	1.697888	-1.812940	-5.865097
C	1.949128	-0.276657	-4.347273
H	2.950892	0.014690	-4.701782
C	1.403485	0.403070	-3.242750
C	-1.906324	-1.579560	-2.842350
H	-2.288664	-0.807103	-2.143879
C	-2.973963	-1.802825	-3.924315
H	-3.135675	-0.894197	-4.538600
H	-3.942469	-2.078727	-3.459679
H	-2.695112	-2.628341	-4.611012
C	-1.666368	-2.860020	-2.022994
H	-0.936015	-2.676567	-1.212255
H	-1.253988	-3.671742	-2.656575
H	-2.611139	-3.219164	-1.566408
C	2.272129	1.456632	-2.555415
H	3.242648	1.411191	-3.095146
C	2.590375	1.113426	-1.091833
H	3.412975	1.748078	-0.703357
H	2.895502	0.057355	-0.960304
H	1.727428	1.340789	-0.414390
C	1.770934	2.905167	-2.679098
H	1.542190	3.169463	-3.730525
H	2.549463	3.607988	-2.316880
H	0.863239	3.075979	-2.068767
N	1.123954	-1.546218	0.582389
C	1.653619	-2.711635	0.655124
C	1.602319	-3.684789	-0.487707
C	1.251592	-5.034912	-0.262407
H	1.045437	-5.371994	0.764909
C	1.153302	-5.936587	-1.331643
H	0.861742	-6.981227	-1.142027
C	1.435801	-5.507240	-2.641570
H	1.376707	-6.217407	-3.480601
C	1.795349	-4.169899	-2.872056
H	2.019245	-3.822718	-3.890883
C	1.861719	-3.260573	-1.807123
H	2.117979	-2.207549	-1.998166
C	2.346316	-3.143841	1.911632
C	1.941693	-2.593223	3.146587
H	1.097746	-1.890448	3.156316
C	2.600810	-2.941263	4.330932
H	2.263166	-2.505288	5.283676
C	3.681088	-3.840202	4.302009
H	4.200657	-4.113034	5.233475
C	4.093212	-4.392012	3.077837
H	4.942129	-5.092422	3.046407
C	3.428129	-4.052155	1.890699
H	3.757225	-4.482350	0.932852

Conformation 28.
Multiplicity: 4
Charge: 0
E(B97-3c) = -3413.540469089547 Hartree
E(M06/def2-TZVP) = -3413.227428110345 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3412.100688568439 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3412.315721314877 Hartree
E(PBEh-3c) = -3408.881497774843 Hartree
E(PM6) = 94.93429 Kcal/mol
E(PM7) = 109.90711 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3415.600531592023 Hartree
E(GFN1-xTB) = -148.540569864825 Hartree
E(GFN2-xTB) = -147.319931789785 Hartree
E(GFN-FF) = -20.504681129888 Hartree

Coordinates:

Co	-0.243746	-0.214629	0.088515
N	0.182779	-1.344777	-1.387044
N	-0.102051	1.501159	-0.863815
C	0.443793	-1.917764	-3.879222
C	0.317346	-0.949778	-2.661128
C	0.290029	0.425021	-2.985848
H	0.420767	0.632785	-4.050013
C	0.130700	1.585747	-2.183786
C	0.267475	2.919210	-3.001755
C	-0.793753	-1.684454	-4.781708
H	-0.751095	-2.359380	-5.661451
H	-0.856907	-0.643712	-5.152600
H	-1.729445	-1.903195	-4.227890
C	1.733458	-1.597556	-4.668887
H	1.813926	-2.275457	-5.543292
H	2.633206	-1.748924	-4.039003
H	1.754359	-0.557590	-5.047191
C	0.471606	-3.420354	-3.544988
H	0.490531	-3.983988	-4.500005
H	-0.421459	-3.747524	-2.982988
H	1.360899	-3.720277	-2.962701
C	1.696691	2.951401	-3.600047
H	1.840722	3.880657	-4.189039
H	1.902057	2.091018	-4.265227
H	2.457448	2.938883	-2.793561
C	0.076677	4.244361	-2.238121
H	0.251244	5.075836	-2.951763
H	0.784241	4.369856	-1.401352
H	-0.941299	4.362658	-1.828149
C	-0.786575	2.918914	-4.137252
H	-0.709610	3.861057	-4.717823
H	-1.811964	2.861813	-3.719360
H	-0.666253	2.078706	-4.847314
C	0.419166	-2.608659	-0.792242
C	1.762406	-3.026629	-0.541663
C	1.967516	-4.250954	0.114010
H	2.996221	-4.594855	0.297585
C	0.889080	-5.033717	0.554010
H	1.072759	-5.988738	1.068172
C	-0.421970	-4.586610	0.347622
H	-1.265826	-5.192723	0.711358
C	-0.685212	-3.380256	-0.325158
C	2.931372	-2.118929	-0.905034
H	2.592071	-1.443244	-1.715886
C	3.289784	-1.223939	0.296988
H	2.398687	-0.684074	0.678663
H	4.056033	-0.472439	0.016345
H	3.685039	-1.828444	1.138653
C	4.159754	-2.876078	-1.424130
H	3.903595	-3.538687	-2.275982
H	4.623841	-3.504018	-0.635838
H	4.936164	-2.162004	-1.765639
C	-2.121481	-2.918878	-0.549888
H	-2.071898	-1.979242	-1.142005
C	-2.824631	-2.595804	0.780435
H	-2.270723	-1.825239	1.353795
H	-2.909608	-3.497791	1.420826
H	-3.848820	-2.211312	0.598728
C	-2.930157	-3.936103	-1.372517
H	-2.449769	-4.150583	-2.348328
H	-3.952496	-3.554319	-1.571104
H	-3.032397	-4.900132	-0.833102
C	-0.404328	2.576848	0.014640
C	-1.755828	3.007908	0.138583
C	-2.049700	4.041382	1.044714
H	-3.088611	4.391726	1.142864
C	-1.047926	4.621576	1.835116
H	-1.296069	5.430961	2.537362
C	0.267081	4.149397	1.739859
H	1.048758	4.589037	2.378658
C	0.614030	3.123925	0.842301
C	-2.871830	2.323759	-0.643422
H	-2.398786	1.755798	-1.470354
C	-3.583949	1.298441	0.259111
H	-2.850863	0.605405	0.720154
H	-4.325047	0.703435	-0.314114
H	-4.116751	1.803564	1.091234
C	-3.865057	3.310790	-1.272096
H	-3.349091	4.052363	-1.915508
H	-4.434102	3.872197	-0.502440
H	-4.605901	2.771452	-1.896849
C	2.054718	2.629214	0.766518
H	2.084599	1.838127	-0.011272
C	2.499420	1.990579	2.092625
H	3.535017	1.601658	2.011450
H	1.837126	1.150662	2.373206
H	2.481640	2.729892	2.919965
C	3.025663	3.746192	0.344736
H	2.743794	4.194712	-0.628659
H	4.059361	3.354074	0.251730
H	3.047886	4.565225	1.093614
N	-0.427489	-0.047351	1.851404
C	-0.403733	-0.283831	3.111920
C	0.667363	-1.132134	3.727495
C	1.158764	-2.253457	3.025794
H	0.716260	-2.511173	2.052986
C	2.186682	-3.036331	3.566228
H	2.543478	-3.916236	3.009961
C	2.752565	-2.702045	4.808005
H	3.560915	-3.317314	5.232757
C	2.278849	-1.580368	5.508834
H	2.724915	-1.306329	6.477404
C	1.237112	-0.805834	4.978842
H	0.866635	0.071840	5.529870
C	-1.465792	0.291448	3.996047
C	-1.942818	-0.398202	5.132383
H	-1.497844	-1.367345	5.404109
C	-2.989465	0.135915	5.898486
H	-3.359451	-0.416388	6.775989
C	-3.563548	1.369409	5.549760
H	-4.379981	1.788959	6.157836

C	-3.084741	2.066518	4.426387
H	-3.516243	3.042090	4.153346
C	-2.050330	1.529403	3.651676
H	-1.668780	2.063266	2.770903

Conformation 29.
Multiplicity: 4
Charge: 0
E(B97-3c) = -3413.522536342741 Hartree
E(M06/def2-TZVP) = -3413.210624300072 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3412.084408221077 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3412.299522016722 Hartree
E(PBEh-3c) = -3408.858963670647 Hartree
E(PM6) = 109.03085 Kcal/mol
E(PM7) = 117.05991 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3415.577131082867 Hartree
E(GFN1-xTB) = -148.524678972839 Hartree
E(GFN2-xTB) = -147.301010405657 Hartree
E(GFN-FF) = -20.489309074126 Hartree

Coordinates:

Co	0.468167	0.107570	0.035649
N	0.026595	-0.762849	-1.689490
N	0.086625	-1.385977	1.185640
C	-0.636223	-2.846635	-3.118885
C	-0.333602	-2.051623	-1.785425
C	-0.470167	-2.861009	-0.624192
H	-0.760389	-3.891447	-0.839979
C	-0.301665	-2.600171	0.754200
C	-0.531859	-3.848046	1.672917
C	-0.431797	-2.087229	-4.443602
H	-0.651248	-2.786724	-5.276446
H	0.601474	-1.721702	-4.576691
H	-1.106611	-1.220233	-4.549121
C	0.273158	-4.103463	-3.179782
H	0.073699	-4.650203	-4.124102
H	0.089801	-4.807803	-2.346591
H	1.344797	-3.834502	-3.167310
C	-2.105872	-3.340257	-3.109518
H	-2.263052	-4.035814	-3.959277
H	-2.818275	-2.502973	-3.236351
H	-2.371630	-3.874399	-2.177233
C	0.488586	-4.934952	1.245888
H	0.365083	-5.834911	1.883016
H	1.527745	-4.567843	1.370981
H	0.367074	-5.246846	0.191270
C	-1.971910	-4.375952	1.470466
H	-2.137223	-5.269695	2.106732
H	-2.175984	-4.666227	0.421977
H	-2.719142	-3.610591	1.760090
C	-0.329576	-3.639053	3.185700
H	-0.451638	-4.621291	3.686402
H	-1.061488	-2.942777	3.630111
H	0.679733	-3.263393	3.431721
C	0.188994	0.152333	-2.759797
C	1.502745	0.368276	-3.284171
C	1.649833	1.198123	-4.409433
H	2.657969	1.341430	-4.830228
C	0.552253	1.846017	-4.990401
H	0.680785	2.471147	-5.886515
C	-0.699025	1.728756	-4.380242
H	-1.555117	2.289439	-4.789033
C	-0.911465	0.922217	-3.241669
C	2.782859	-0.213551	-2.676614
H	3.599302	0.286233	-3.241539
C	3.009268	0.170489	-1.207300
H	2.807746	1.240545	-1.017928
H	4.051911	-0.053544	-0.901378
H	2.379282	-0.454983	-0.521176
C	2.983153	-1.723795	-2.869026
H	2.821437	-2.030876	-3.921176
H	2.295206	-2.304053	-2.224906
H	4.018326	-2.009863	-2.589359
C	-2.306428	1.054270	-2.608167
H	-3.011684	1.067761	-3.470265
C	-2.422033	2.432317	-1.919135
H	-2.113270	3.258857	-2.588516
H	-1.776081	2.467191	-1.021778
H	-3.467728	2.616892	-1.597787
C	-2.809613	-0.026737	-1.645987
H	-2.828418	-1.031718	-2.098773
H	-3.845041	0.220819	-1.335299
H	-2.190171	-0.088519	-0.733379
C	0.099619	-0.893696	2.518761
C	1.342278	-0.712446	3.191840
C	1.334192	-0.198746	4.501036
H	2.289343	-0.068271	5.033183
C	0.135257	0.135887	5.142257
H	0.146516	0.518384	6.174207
C	-1.077151	0.002782	4.451315
H	-2.014896	0.306233	4.940689
C	-1.122980	-0.491913	3.138431
C	2.665351	-1.039816	2.511625
H	2.420037	-1.510871	1.536983
C	3.448297	0.254821	2.228737
H	2.834905	0.970464	1.643999
H	4.375557	0.047377	1.656536
H	3.739295	0.759159	3.173391
C	3.511243	-2.046505	3.306530
H	2.958986	-2.991788	3.481351
H	3.806273	-1.642131	4.296767
H	4.443334	-2.293341	2.757891
C	-2.444515	-0.523193	2.379217
H	-2.305682	-1.174881	1.493354
C	-2.771795	0.890530	1.863291
H	-3.692507	0.885696	1.245623
H	-1.941554	1.287662	1.246273
H	-2.917952	1.596676	2.706300
C	-3.607210	-1.103058	3.197015
H	-3.367239	-2.108008	3.599887
H	-4.512823	-1.195945	2.563552
H	-3.877076	-0.453356	4.055147
N	0.487904	1.896371	-0.048887
C	0.417677	3.140020	0.251440
C	-0.291697	3.606056	1.491077
C	-0.038327	2.995316	2.736094
H	0.710190	2.191511	2.803306
C	-0.734107	3.406864	3.881368
H	-0.511518	2.930075	4.846801
C	-1.715517	4.407358	3.793395
H	-2.267140	4.721871	4.692625
C	-1.990431	5.005696	2.552415
H	-2.765782	5.783342	2.473429
C	-1.273149	4.618764	1.411781
H	-1.479470	5.093657	0.440432
C	1.014085	4.171748	-0.656052
C	1.238451	3.847008	-2.012498
H	0.936119	2.854045	-2.371320
C	1.821917	4.775447	-2.881005
H	1.975312	4.502977	-3.936720
C	2.200023	6.044962	-2.409430
H	2.658994	6.776577	-3.092134
C	1.986363	6.376533	-1.061550
H	2.285704	7.366278	-0.683371
C	1.394384	5.450033	-0.190196
H	1.234737	5.713327	0.866018

Conformation 6.
Multiplicity: 4
Charge: 0
E(B97-3c) = -3413.532685288374 Hartree
E(M06/def2-TZVP) = -3413.222124048085 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3412.094209379966 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3412.308342631976 Hartree
E(PBEh-3c) = -3408.870757868448 Hartree
E(PM6) = 99.67616 Kcal/mol
E(PM7) = 114.02554 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3415.589059046359 Hartree
E(GFN1-xTB) = -148.535057129350 Hartree
E(GFN2-xTB) = -147.313145160225 Hartree
E(GFN-FF) = -20.500698107896 Hartree

Coordinates:

Co	0.007013	0.251105	-0.055104
N	0.505242	-1.536927	-0.711237
N	1.148615	0.291787	1.474187
C	2.079556	-3.607236	-0.718265
C	1.524447	-2.236812	-0.179045
C	2.239800	-1.764932	0.952926
H	3.067312	-2.410069	1.256747
C	2.118988	-0.592049	1.735336
C	3.226605	-0.405489	2.821053
C	1.309237	-4.274197	-1.875518
H	1.792597	-5.249953	-2.087189
H	1.326397	-3.682998	-2.807119
H	0.251761	-4.471800	-1.627088
C	3.530416	-3.379141	-1.210577
H	3.955323	-4.335613	-1.579214
H	4.194023	-2.999984	-0.409641
H	3.559861	-2.652343	-2.045039
C	2.099873	-4.635825	0.442524
H	2.467469	-5.611194	0.063412
H	1.085428	-4.791730	0.858400
H	2.760803	-4.335004	1.277074
C	4.586390	-0.327961	2.080833
H	5.406891	-0.173310	2.811580
H	4.596865	0.521299	1.368017
H	4.808001	-1.248225	1.507383
C	3.225329	-1.617816	3.780913
H	4.024682	-1.496022	4.540571
H	3.402457	-2.577472	3.258852
H	2.258668	-1.698626	4.318183

C	3.112723	0.862827	3.687164
H	4.000929	0.909359	4.349620
H	2.216826	0.863255	4.333097
H	3.093442	1.792277	3.090028
C	-0.165167	-1.823712	-1.933732
C	0.430437	-1.365440	-3.149399
C	-0.222175	-1.618923	-4.367571
H	0.239005	-1.275952	-5.306190
C	-1.448827	-2.293317	-4.404169
H	-1.946761	-2.495580	-5.364238
C	-2.045017	-2.687732	-3.202115
H	-3.022168	-3.196771	-3.222591
C	-1.440551	-2.459028	-1.948853
C	1.720999	-0.551122	-3.142352
H	2.197725	-0.685904	-2.150647
C	2.731157	-1.005882	-4.206362
H	2.938293	-2.093142	-4.141014
H	3.691924	-0.465154	-4.084234
H	2.369887	-0.796927	-5.234363
C	1.401059	0.949056	-3.290636
H	0.660053	1.274317	-2.532238
H	0.961842	1.164507	-4.286862
H	2.318600	1.564045	-3.178659
C	-2.272358	-2.858550	-0.724001
H	-2.942617	-3.665145	-1.095357
C	-3.181990	-1.692751	-0.292988
H	-3.769460	-1.298351	-1.145410
H	-2.575774	-0.853878	0.098489
H	-3.886293	-2.014756	0.501416
C	-1.538251	-3.439846	0.492045
H	-0.869825	-4.276483	0.211905
H	-2.281589	-3.835002	1.214504
H	-0.932177	-2.678929	1.017443
C	0.723738	1.446129	2.172981
C	0.955264	2.729293	1.590717
C	0.458567	3.865367	2.254737
H	0.640129	4.861267	1.822944
C	-0.261978	3.752112	3.449933
H	-0.635310	4.653802	3.957892
C	-0.529010	2.481422	3.982676
H	-1.124021	2.396231	4.903932
C	-0.066134	1.313661	3.356718
C	1.730686	2.879647	0.285226
H	1.825991	1.858657	-0.156294
C	0.989838	3.754470	-0.737208
H	-0.025889	3.360041	-0.936126
H	1.540004	3.774444	-1.699417
H	0.893954	4.802877	-0.388043
C	3.159883	3.392207	0.532244
H	3.722607	2.726056	1.215808
H	3.140324	4.403010	0.990361
H	3.724491	3.461231	-0.420236
C	-0.455647	-0.068770	3.865886
H	0.346968	-0.771939	3.564634
C	-1.743197	-0.533729	3.160311
H	-1.980612	-1.587091	3.413789
H	-1.642606	-0.461159	2.058795
H	-2.605880	0.100694	3.448165
C	-0.592388	-0.155360	5.390300
H	0.320960	0.204799	5.906443
H	-0.770739	-1.204713	5.700683
H	-1.450150	0.441247	5.763658
N	-1.373514	0.992668	-0.903941
C	-2.450155	1.643992	-1.150019
C	-3.415855	1.982501	-0.054999
C	-2.930366	2.346612	1.218987
H	-1.845470	2.427663	1.375856
C	-3.817865	2.613797	2.269205
H	-3.417024	2.914188	3.249151
C	-5.204068	2.501860	2.070251
H	-5.901066	2.706837	2.897298
C	-5.697385	2.130286	0.808529
H	-6.782024	2.032656	0.646958
C	-4.811734	1.883145	-0.249990
H	-5.200361	1.592488	-1.237685
C	-2.769244	2.053012	-2.554081
C	-3.488974	3.232726	-2.845991
H	-3.855044	3.863305	-2.021760
C	-3.721246	3.611529	-4.176583
H	-4.273512	4.539415	-4.391441
C	-3.250539	2.813079	-5.231801
H	-3.440832	3.108673	-6.275051
C	-2.538918	1.634061	-4.948440
H	-2.174268	0.995066	-5.767860
C	-2.295068	1.260161	-3.622280
H	-1.739261	0.341545	-3.390509

ROBHUN

Conformation 10.

Multiplicity: 5
Charge: 0
E(B97-3c) = -5596.386662097501 Hartree
E(M06/def2-TZVP) = -5596.635267331795 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -5594.599066129174 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -5594.995838439150 Hartree
E(PBEh-3c) = -5589.624015247439 Hartree
E(PM6) = -2.72851 Kcal/mol
E(PM7) = 107.91092 Kcal/mol
E(ωB97X-V/def2-TZVP) = -5597.233921337914 Hartree
E(GFN1-xTB) = -152.461249225203 Hartree
E(GFN2-xTB) = -152.110505793784 Hartree
E(GFN-FF) = -19.124830578190 Hartree

Coordinates:

Cr	0.291712	-0.318149	-0.695226
Al	-1.281855	4.319588	0.898640
Cl	1.864300	-0.598462	-2.344844
Cl	-1.083540	4.500465	3.083910
Cl	0.207347	5.573835	-0.059247
N	-2.364441	-1.910997	-0.356539
H	-3.165912	-2.546264	-0.336617
N	-1.496735	0.192913	0.235627
N	-0.748368	2.446158	0.542139
P	-1.052148	-2.118690	-1.468742
P	0.545103	2.015747	-0.522931
P	1.533467	-1.234139	1.320476
C	-2.498111	-0.733003	0.367642
C	-3.600532	-0.529492	1.212003
H	-4.383993	-1.294981	1.292187
C	-3.634860	0.651449	1.969255
H	-4.451562	0.816661	2.687915
C	-2.652041	1.625604	1.812704
H	-2.656872	2.547420	2.409486
C	-1.615251	1.428376	0.860846
C	-0.584736	-3.867759	-1.266398
C	-0.823394	-4.562137	-0.063397
H	-1.384179	-4.080913	0.751466
C	-0.317553	-5.859983	0.104269
H	-0.508276	-6.394227	1.046905
C	0.438403	-6.462462	-0.913461
H	0.838733	-7.478215	-0.775320
C	0.688252	-5.765345	-2.107973
H	1.286529	-6.231342	-2.905341
C	0.181005	-4.472029	-2.287988
H	0.389509	-3.920219	-3.217624
C	-1.760213	-2.005242	-3.154513
C	-1.468553	-0.844624	-3.899986
H	-0.765369	-0.099099	-3.494275
C	-2.054885	-0.659809	-5.160942
H	-1.821666	0.247594	-5.738488
C	-2.927841	-1.629567	-5.678552
H	-3.387825	-1.483828	-6.667886
C	-3.210796	-2.793171	-4.941201
H	-3.888832	-3.555939	-5.353411
C	-2.626188	-2.986030	-3.681773
H	-2.835455	-3.904647	-3.110411
C	2.138783	2.578138	0.155613
C	2.253607	3.342143	1.331899
H	1.360298	3.666798	1.882358
C	3.526192	3.677768	1.814679
H	3.608693	4.274108	2.735169
C	4.680879	3.259854	1.135667
H	5.675498	3.533449	1.520069
C	4.566132	2.480710	-0.026924
H	5.467693	2.136344	-0.556394
C	3.299532	2.128226	-0.514673
H	3.203820	1.481235	-1.401485
C	0.229737	2.887260	-2.100358
C	1.193807	3.663869	-2.766488
H	2.170448	3.847482	-2.296086
C	0.891979	4.226375	-4.014989
H	1.645853	4.840800	-4.529971
C	-0.369059	4.025469	-4.598528
H	-0.602782	4.476780	-5.574735
C	-1.335676	3.255309	-3.930239
H	-2.330208	3.102157	-4.376603
C	-1.036153	2.679966	-2.687923
H	-1.791378	2.070205	-2.167091
C	-3.095137	4.652149	0.187094
H	-3.036711	4.467243	-0.910833
H	-3.824933	3.908143	0.575501
C	-3.593614	6.081255	0.454705
H	-4.591524	6.287302	0.007757
H	-2.889820	6.836095	0.044492
H	-3.676018	6.283993	1.543792
C	2.006283	-0.000015	2.610672
C	3.328510	0.159596	3.070931
H	4.146712	-0.442104	2.651196
C	3.617181	1.095785	4.076334
H	4.655060	1.211416	4.424188

C	2.597002	1.884375	4.628465
H	2.830289	2.622414	5.410780
C	1.281543	1.749591	4.157882
H	0.478086	2.399774	4.534188
C	0.990903	0.816206	3.154955
H	-0.042011	0.743068	2.786887
C	0.620775	-2.474009	2.345870
C	1.176734	-3.706176	2.745997
H	2.210294	-3.965839	2.477963
C	0.417541	-4.620700	3.492965
H	0.867203	-5.579147	3.794892
C	-0.903317	-4.317070	3.858205
H	-1.495551	-5.036907	4.443280
C	-1.458249	-3.082439	3.482210
H	-2.488045	-2.822068	3.771160
C	-0.703801	-2.171622	2.730557
H	-1.155221	-1.212707	2.443645
C	3.116448	-2.076063	0.857735
H	3.738233	-1.265957	0.421230
H	3.630034	-2.426645	1.778220
C	2.926841	-3.199948	-0.165883
H	3.900848	-3.679984	-0.389681
H	2.522777	-2.789349	-1.110991
H	2.234580	-3.989146	0.188292

Conformation 12.
Multiplicity: 5
Charge: 0
E(B97-3c) = -5596.388741295847 Hartree
E(M06/def2-TZVP) = -5596.637594551751 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -5594.601050021001 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -5594.997897810705 Hartree
E(PBEh-3c) = -5589.628078717655 Hartree
E(PM6) = -6.68397 Kcal/mol
E(PM7) = 98.27049 Kcal/mol
E(ωB97X-V/def2-TZVP) = -5597.236224588247 Hartree
E(GFN1-xTB) = -152.466692943338 Hartree
E(GFN2-xTB) = -152.117532403262 Hartree
E(GFN-FF) = -19.125123480387 Hartree

Coordinates:

Cr	0.656844	-0.379961	-0.274018
Al	-4.161846	-0.434672	1.533698
Cl	1.473327	-1.631865	-2.018105
Cl	-4.957010	1.599257	1.255293
Cl	-5.121756	-1.747188	0.091895
N	2.217869	0.604282	2.237960
H	2.839195	0.806981	3.025369
N	-0.020489	0.314123	1.563266
N	-2.271542	-0.233928	0.970368
P	2.717882	-0.398610	0.919351
P	-1.555925	-1.202514	-0.274614
P	0.541348	1.924465	-1.295092
C	0.860636	0.832612	2.472878
C	0.444902	1.568158	3.589012
H	1.184771	1.975574	4.291100
C	-0.931520	1.792032	3.747771
H	-1.293638	2.407404	4.584625
C	-1.845276	1.236667	2.860118
H	-2.920481	1.429788	2.961517
C	-1.384078	0.436500	1.781142
C	4.283115	0.368345	0.377549
C	4.701681	1.644539	0.803723
H	4.097823	2.203652	1.534536
C	5.878472	2.206362	0.283625
H	6.204197	3.200920	0.624154
C	6.634226	1.505113	-0.668785
H	7.554478	1.949305	-1.077036
C	6.211034	0.237676	-1.104810
H	6.794802	-0.310232	-1.859659
C	5.039893	-0.330897	-0.588254
H	4.696043	-1.314461	-0.945381
C	3.251791	-2.012092	1.613446
C	4.349800	-2.133271	2.490442
H	4.972214	-1.254280	2.723884
C	4.654758	-3.379127	3.055536
H	5.508267	-3.475034	3.743814
C	3.875621	-4.506577	2.738703
H	4.120268	-5.482969	3.184060
C	2.795618	-4.391761	1.849800
H	2.188789	-5.272371	1.590099
C	2.482287	-3.146162	1.284671
H	1.649408	-3.047116	0.569508
C	-2.446392	-0.914666	-1.831447
C	-2.117095	-1.729619	-2.936492
H	-1.359300	-2.520986	-2.832695
C	-2.741750	-1.512458	-4.172069
H	-2.494278	-2.159923	-5.027055
C	-3.661818	-0.462602	-4.322812
H	-4.142442	-0.287257	-5.297149
C	-3.955337	0.373143	-3.234576
H	-4.669184	1.202307	-3.347990
C	-3.356632	0.148910	-1.987675
H	-3.625401	0.784444	-1.130360
C	-1.804390	-2.948697	0.230575
C	-2.614707	-3.875453	-0.451376
H	-3.188841	-3.558920	-1.332642
C	-2.711213	-5.193879	0.017912
H	-3.350128	-5.914305	-0.515066
C	-2.016239	-5.591252	1.171020
H	-2.102699	-6.625524	1.537448
C	-1.218268	-4.664635	1.862550
H	-0.679111	-4.965521	2.773778
C	-1.107559	-3.349837	1.390653
H	-0.477654	-2.623221	1.927870
C	-4.266559	-1.153076	3.377356
H	-3.389011	-0.805424	3.967420
H	-5.148954	-0.680962	3.866364
C	-4.377314	-2.684916	3.451976
H	-4.479652	-3.058172	4.495178
H	-3.486092	-3.184260	3.016090
H	-5.250276	-3.058098	2.877950
C	-0.345715	2.155200	-2.888147
C	-0.299641	1.097543	-3.820203
H	0.191126	0.150078	-3.545177
C	-0.887899	1.253985	-5.083790
H	-0.853024	0.422716	-5.803296
C	-1.538943	2.450933	-5.418584
H	-2.011135	2.565046	-6.406358
C	-1.596850	3.500556	-4.487290
H	-2.111449	4.439433	-4.743387
C	-0.996727	3.359556	-3.227663
H	-1.041661	4.185528	-2.502070
C	-0.214163	3.147939	-0.156958
C	0.563287	4.029920	0.623588
H	1.656995	4.056190	0.511733
C	-0.053224	4.888683	1.547071
H	0.565092	5.575069	2.145939
C	-1.447643	4.877889	1.703063
H	-1.928168	5.556537	2.424042
C	-2.227646	3.993874	0.940321
H	-3.317958	3.938767	1.074050
C	-1.615535	3.130393	0.023471
H	-2.238089	2.430389	-0.552792
C	2.227326	2.625314	-1.665837
H	2.108869	3.695717	-1.936639
H	2.785595	2.577580	-0.709041
C	2.968037	1.840424	-2.747816
H	4.014822	2.194317	-2.829976
H	2.483831	1.963098	-3.736700
H	2.986025	0.755546	-2.521727

Conformation 13.
Multiplicity: 5
Charge: 0
E(B97-3c) = -5596.381461906616 Hartree
E(M06/def2-TZVP) = -5596.630859369398 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -5594.594213748065 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -5594.990841260730 Hartree
E(PBEh-3c) = -5589.618818048475 Hartree
E(PM6) = 3.63514 Kcal/mol
E(PM7) = 116.33626 Kcal/mol
E(ωB97X-V/def2-TZVP) = -5597.229013990561 Hartree
E(GFN1-xTB) = -152.460005404970 Hartree
E(GFN2-xTB) = -152.111342636979 Hartree
E(GFN-FF) = -19.126197386254 Hartree

Coordinates:

Cr	0.250465	-0.792403	-0.175308
Al	-4.125790	0.766571	2.101154
Cl	0.493616	-2.700074	-1.421508
Cl	-5.360680	-0.980705	1.721512
Cl	-3.725832	0.990590	4.226497
N	2.335674	0.857313	1.371403
H	3.153909	1.377705	1.693786
N	0.000391	0.736471	1.194524
N	-2.356262	0.339743	1.301324
P	2.414746	-0.795275	0.856479
P	-1.971231	-1.172336	0.530152
P	0.610465	0.755561	-2.122015
C	1.098554	1.449465	1.598135
C	0.988567	2.694173	2.231142
H	1.889703	3.249671	2.524133
C	-0.304174	3.167929	2.510163
H	-0.435378	4.141269	3.005806
C	-1.423870	2.401201	2.208271
H	-2.423247	2.746089	2.490157
C	-1.270167	1.144310	1.566235
C	3.987028	-0.961871	-0.058967
C	5.186723	-0.369190	0.383052
H	5.209825	0.236330	1.303052
C	6.369530	-0.561246	-0.343107

H	7.303089	-0.088180	-0.002979
C	6.366015	-1.368798	-1.493524
H	7.300046	-1.528122	-2.053719
C	5.175980	-1.973806	-1.924567
H	5.171509	-2.608044	-2.824007
C	3.980905	-1.763248	-1.218672
H	3.032420	-2.214367	-1.557429
C	2.708221	-1.750533	2.396819
C	2.269690	-1.253785	3.642011
H	1.859444	-0.235195	3.716915
C	2.349290	-2.061675	4.786559
H	2.007299	-1.666968	5.755223
C	2.857235	-3.367659	4.695184
H	2.915329	-4.000421	5.593588
C	3.288217	-3.866218	3.453996
H	3.684688	-4.890019	3.378255
C	3.213071	-3.065132	2.306631
H	3.544706	-3.462537	1.334637
C	-3.141916	-1.449789	-0.833194
C	-3.064733	-2.683087	-1.517286
H	-2.377610	-3.467040	-1.166110
C	-3.840189	-2.894562	-2.665920
H	-3.777534	-3.859269	-3.191748
C	-4.680937	-1.879297	-3.150454
H	-5.284830	-2.047595	-4.055003
C	-4.747728	-0.648709	-2.478064
H	-5.406947	0.151180	-2.847311
C	-3.984238	-0.433055	-1.323221
H	-4.051546	0.527458	-0.794752
C	-2.131729	-2.535288	1.739490
C	-1.065370	-2.660881	2.655174
H	-0.221317	-1.954463	2.610370
C	-1.066741	-3.689581	3.604907
H	-0.228119	-3.774085	4.312416
C	-2.126792	-4.610824	3.631943
H	-2.128642	-5.426173	4.371516
C	-3.183064	-4.495259	2.713664
H	-4.016188	-5.213866	2.738561
C	-3.194176	-3.457783	1.769767
H	-4.034576	-3.348874	1.070985
C	-5.023967	2.352115	1.299487
H	-5.069743	2.235949	0.191175
H	-6.077495	2.183965	1.623642
C	-4.608021	3.782656	1.668784
H	-5.339702	4.548640	1.328920
H	-3.629768	4.062984	1.223423
H	-4.505758	3.901369	2.768831
C	-0.492392	2.218381	-2.311518
C	-1.687948	2.277959	-1.572818
H	-1.936889	1.470471	-0.871950
C	-2.566837	3.362002	-1.728366
H	-3.494463	3.398629	-1.137788
C	-2.253253	4.393686	-2.624939
H	-2.938647	5.246452	-2.745007
C	-1.060514	4.340328	-3.367945
H	-0.812457	5.149165	-4.072236
C	-0.181777	3.259635	-3.212980
H	0.757209	3.227175	-3.787420
C	2.277030	1.529945	-2.136994
C	2.516839	2.644651	-1.301413
H	1.686377	3.087352	-0.729492
C	3.801191	3.194814	-1.202683
H	3.970451	4.068334	-0.553824
C	4.866868	2.640590	-1.932774
H	5.876358	3.071521	-1.853334
C	4.635336	1.538719	-2.769094
H	5.462974	1.097239	-3.343870
C	3.350150	0.984222	-2.870760
H	3.189285	0.112761	-3.521157
C	0.463127	-0.105166	-3.761541
H	0.850956	0.571094	-4.552640
H	1.125176	-0.993219	-3.689796
C	-0.975748	-0.548591	-4.028026
H	-1.042725	-1.074827	-5.001145
H	-1.673681	0.311795	-4.056808
H	-1.322347	-1.248536	-3.242667

Conformation 14.
Multiplicity: 5
Charge: 0
E(B97-3c) = -5596.391804898873 Hartree
E(M06/def2-TZVP) = -5596.639195694533 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -5594.603531118059 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -5595.000697110750 Hartree
E(PBEh-3c) = -5589.630706915516 Hartree
E(PM6) = -6.75326 Kcal/mol
E(PM7) = 102.32169 Kcal/mol
E(ωB97X-V/def2-TZVP) = -5597.238714056441 Hartree
E(GFN1-xTB) = -152.466465307826 Hartree
E(GFN2-xTB) = -152.118048322471 Hartree
E(GFN-FF) = -19.123985372431 Hartree

Coordinates:

Cr	-0.607837	0.188841	0.392782
Al	4.408126	1.392755	0.460482
Cl	-2.283937	1.457888	1.318251
Cl	5.175090	1.533398	-1.596487
Cl	4.306360	3.393582	1.302840
N	-0.394205	-2.922169	0.282482
H	-0.462643	-3.941699	0.336354
N	1.032814	-1.064697	0.089690
N	2.536289	0.790138	0.215871
P	-1.607128	-1.900671	0.979670
P	1.186570	1.659592	0.847923
P	-1.033162	0.626000	-2.038400
C	0.860815	-2.415280	-0.041582
C	1.879989	-3.266856	-0.488921
H	1.700606	-4.347423	-0.570790
C	3.097941	-2.683943	-0.868449
H	3.899738	-3.310979	-1.286004
C	3.304807	-1.317720	-0.715645
H	4.242185	-0.841358	-1.030229
C	2.283069	-0.513135	-0.146950
C	-3.140036	-2.634534	0.313459
C	-3.142003	-3.342756	-0.905569
H	-2.197459	-3.499425	-1.447401
C	-4.345347	-3.834020	-1.430112
H	-4.338459	-4.385067	-2.382260
C	-5.553797	-3.611003	-0.752013
H	-6.497530	-3.995956	-1.166917
C	-5.558634	-2.884242	0.450063
H	-6.505208	-2.698369	0.979812
C	-4.358674	-2.393171	0.982951
H	-4.364548	-1.822380	1.924367
C	-1.668217	-2.277363	2.774832
C	-2.088087	-3.527156	3.276923
H	-2.481077	-4.295067	2.591414
C	-2.013995	-3.785315	4.652598
H	-2.338108	-4.761094	5.045430
C	-1.529561	-2.798545	5.530094
H	-1.474555	-3.006167	6.609666
C	-1.123985	-1.549712	5.034062
H	-0.750873	-0.770386	5.715685
C	-1.193144	-1.286430	3.657744
H	-0.890586	-0.304007	3.259180
C	1.093714	3.265148	-0.004414
C	1.969758	3.606219	-1.055241
H	2.797015	2.936558	-1.333956
C	1.777295	4.806084	-1.755446
H	2.468414	5.069819	-2.570082
C	0.721695	5.667888	-1.414118
H	0.579443	6.610020	-1.965069
C	-0.155879	5.322477	-0.373446
H	-0.994597	5.985643	-0.112952
C	0.017917	4.118628	0.324937
H	-0.703093	3.819465	1.101686
C	1.528555	1.947500	2.624205
C	1.513425	3.212748	3.238196
H	1.368336	4.117101	2.630587
C	1.721730	3.318235	4.620868
H	1.716965	4.310854	5.095951
C	1.958406	2.170111	5.393467
H	2.130896	2.260943	6.476654
C	1.985792	0.906462	4.780001
H	2.183360	0.002809	5.376712
C	1.762593	0.792781	3.401050
H	1.778063	-0.199054	2.921904
C	5.364906	0.144353	1.656010
H	4.793759	0.141146	2.613692
H	5.312052	-0.899106	1.275320
C	6.825210	0.547165	1.915676
H	7.342290	-0.125361	2.635704
H	6.891882	1.577342	2.325060
H	7.420780	0.539747	0.977979
C	0.343070	-0.076947	-3.021532
C	0.401034	-1.466099	-3.272006
H	-0.441592	-2.110949	-2.977913
C	1.526116	-2.028252	-3.889471
H	1.555061	-3.111440	-4.082721
C	2.622086	-1.220919	-4.234970
H	3.514198	-1.668274	-4.698405
C	2.585581	0.154910	-3.964815
H	3.454924	0.789887	-4.187957
C	1.451061	0.725899	-3.370035
H	1.446465	1.803648	-3.154687
C	-2.581171	-0.124688	-2.688667
C	-3.709843	-0.094637	-1.839568
H	-3.607468	0.294967	-0.813041
C	-4.951613	-0.550921	-2.303845
H	-5.824924	-0.519612	-1.635863
C	-5.073234	-1.066661	-3.603595
H	-6.045943	-1.437539	-3.961403

C	-3.950652	-1.111736	-4.446544
H	-4.042694	-1.511808	-5.468125
C	-2.710441	-0.632252	-3.997765
H	-1.838488	-0.651028	-4.669217
C	-1.177867	2.387056	-2.632459
H	-0.266659	2.905367	-2.274383
H	-1.144388	2.367736	-3.742486
C	-2.428472	3.090738	-2.107826
H	-2.403481	4.162092	-2.390446
H	-2.488872	3.027039	-1.003099
H	-3.354084	2.646601	-2.524987

Conformation 19.
Multiplicity: 5
Charge: 0
E(B97-3c) = -5596.387477016558 Hartree
E(M06/def2-TZVP) = -5596.635339660322 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -5594.599477123957 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -5594.995563611253 Hartree
E(PBEh-3c) = -5589.622642189024 Hartree
E(PM6) = -0.77869 Kcal/mol
E(PM7) = 114.46982 Kcal/mol
E(ωB97X-V/def2-TZVP) = -5597.232967487661 Hartree
E(GFN1-xTB) = -152.457780957736 Hartree
E(GFN2-xTB) = -152.110266014246 Hartree
E(GFN-FF) = -19.097472231007 Hartree

Coordinates:

Cr	0.200994	0.130735	0.478513
Al	2.569220	-3.159814	-2.701227
Cl	1.321595	1.431955	1.989730
Cl	1.955744	-2.716336	-4.759525
Cl	4.604405	-2.481540	-2.381178
N	-2.383548	-1.491453	1.085562
H	-3.246383	-1.930378	1.416234
N	-0.558688	-1.598024	-0.392419
N	1.459272	-1.908440	-1.639487
P	-1.462414	-0.397439	2.065064
P	2.104997	-0.650091	-0.650570
P	-0.683444	1.884797	-1.110424
C	-1.797372	-2.065107	-0.037940
C	-2.460604	-3.058337	-0.773935
H	-3.453470	-3.408466	-0.460870
C	-1.825699	-3.556366	-1.922997
H	-2.338298	-4.297781	-2.554066
C	-0.543776	-3.134372	-2.265534
H	-0.041437	-3.503947	-3.169098
C	0.129802	-2.200073	-1.434959
C	-2.675253	0.834649	2.630168
C	-3.834322	1.128347	1.883145
H	-4.084816	0.530613	0.993944
C	-4.648499	2.207718	2.256786
H	-5.549807	2.430922	1.666843
C	-4.305305	3.006814	3.358613
H	-4.942992	3.857594	3.642417
C	-3.141833	2.724058	4.094890
H	-2.865569	3.352465	4.955116
C	-2.325355	1.643404	3.735454
H	-1.402717	1.434589	4.298351
C	-0.942640	-1.311164	3.563582
C	-1.839566	-1.668390	4.591705
H	-2.887272	-1.329504	4.554215
C	-1.389104	-2.445499	5.668211
H	-2.087167	-2.726135	6.471606
C	-0.046997	-2.861607	5.723633
H	0.302309	-3.469303	6.572375
C	0.848970	-2.497447	4.705859
H	1.903057	-2.811039	4.749106
C	0.405417	-1.721396	3.625378
H	1.106867	-1.412091	2.832928
C	2.901678	0.624638	-1.687960
C	3.158927	1.867854	-1.063023
H	2.918620	2.007423	0.004044
C	3.664594	2.937756	-1.816323
H	3.857291	3.902581	-1.323160
C	3.894603	2.783578	-3.193614
H	4.282323	3.626227	-3.786451
C	3.615954	1.555356	-3.815544
H	3.781813	1.430003	-4.896191
C	3.122191	0.473182	-3.071447
H	2.883773	-0.469055	-3.584794
C	3.339306	-1.413906	0.456005
C	4.493255	-0.728150	0.876559
H	4.749596	0.243937	0.431093
C	5.326710	-1.300149	1.847957
H	6.234335	-0.765931	2.167342
C	5.014542	-2.550735	2.404828
H	5.675666	-2.996921	3.163142
C	3.861394	-3.234833	1.984988
H	3.617205	-4.222102	2.406239
C	3.019837	-2.667121	1.018719
H	2.119498	-3.206123	0.685277
C	2.217915	-5.018282	-2.102469
H	3.169192	-5.373346	-1.645572
H	1.486891	-4.985758	-1.261565
C	1.743823	-6.014866	-3.169758
H	1.600700	-7.042990	-2.769293
H	2.464147	-6.089580	-4.010778
H	0.776599	-5.708090	-3.622430
C	-2.511310	1.767033	-1.347232
C	-3.387092	2.857538	-1.169843
H	-2.985454	3.840278	-0.882608
C	-4.769621	2.690833	-1.344831
H	-5.441893	3.550871	-1.201398
C	-5.295869	1.438522	-1.701370
H	-6.380901	1.312034	-1.836053
C	-4.428210	0.350107	-1.892329
H	-4.824930	-0.636277	-2.177940
C	-3.046934	0.511336	-1.712596
H	-2.380299	-0.350555	-1.855445
C	-0.433074	3.558439	-0.408313
C	0.285444	4.574866	-1.068778
H	0.693591	4.408010	-2.075418
C	0.496150	5.813062	-0.439770
H	1.061719	6.598620	-0.963931
C	-0.012428	6.050236	0.845888
H	0.153751	7.022296	1.334555
C	-0.724826	5.037957	1.510956
H	-1.117511	5.207614	2.525091
C	-0.921386	3.796035	0.896391
H	-1.454726	3.000287	1.436763
C	-0.065781	2.014565	-2.863818
H	-0.583699	2.877496	-3.333196
H	1.010179	2.269364	-2.780663
C	-0.242149	0.744195	-3.694170
H	0.221993	0.879323	-4.691211
H	-1.309649	0.496098	-3.855088
H	0.254239	-0.131904	-3.234662

Conformation 29.
Multiplicity: 5
Charge: 0
E(B97-3c) = -5596.389669026221 Hartree
E(M06/def2-TZVP) = -5596.638730052295 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -5594.601785706922 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -5594.999421417705 Hartree
E(PBEh-3c) = -5589.628270586791 Hartree
E(PM6) = -3.43148 Kcal/mol
E(PM7) = 116.09397 Kcal/mol
E(ωB97X-V/def2-TZVP) = -5597.237306392426 Hartree
E(GFN1-xTB) = -152.466153330815 Hartree
E(GFN2-xTB) = -152.114335810143 Hartree
E(GFN-FF) = -19.131015148398 Hartree

Coordinates:

Cr	0.137706	-0.643828	0.213450
Al	-1.477923	2.050779	-3.849012
Cl	1.288344	-2.626509	0.122526
Cl	-3.611179	2.374316	-3.544760
Cl	-0.399593	3.975192	-3.890985
N	-1.814018	0.387719	2.403544
H	-2.423369	0.611919	3.192872
N	-1.184244	0.952616	0.209564
N	-0.873858	1.272507	-2.133754
P	-1.160654	-1.198610	2.149099
P	-0.164571	-0.301338	-2.109950
P	2.043143	0.667158	1.223288
C	-1.807472	1.319445	1.372993
C	-2.413938	2.574574	1.524662
H	-2.893401	2.844816	2.475312
C	-2.374227	3.457804	0.434495
H	-2.805378	4.465270	0.531892
C	-1.823063	3.065673	-0.781954
H	-1.803883	3.741434	-1.645288
C	-1.284250	1.761193	-0.910361
C	-0.461243	-1.681717	3.762077
C	0.540921	-2.675972	3.734958
H	0.895274	-3.061112	2.763957
C	1.092248	-3.141448	4.936917
H	1.874356	-3.915397	4.912758
C	0.654300	-2.619568	6.165223
H	1.088363	-2.987827	7.107213
C	-0.329293	-1.618661	6.191088
H	-0.661259	-1.193779	7.150361
C	-0.885583	-1.146645	4.993135
H	-1.639799	-0.346496	5.030163
C	-2.603914	-2.310294	1.923615
C	-3.292233	-2.930675	2.985502
H	-2.948399	-2.793586	4.022580
C	-4.409302	-3.734908	2.714248
H	-4.946658	-4.220870	3.542891
C	-4.836702	-3.928307	1.389495

H	-5.710035	-4.565607	1.182985
C	-4.144089	-3.321554	0.328843
H	-4.461554	-3.478451	-0.713303
C	-3.026614	-2.519153	0.593871
H	-2.466359	-2.056415	-0.235575
C	1.384160	-0.247162	-3.077045
C	1.854007	0.934293	-3.685905
H	1.261645	1.861661	-3.655091
C	3.093679	0.935843	-4.341045
H	3.450059	1.864383	-4.811750
C	3.868422	-0.233218	-4.400861
H	4.838576	-0.226664	-4.920556
C	3.408264	-1.407706	-3.784318
H	4.020173	-2.322179	-3.807291
C	2.178782	-1.415828	-3.110008
H	1.858895	-2.314914	-2.561014
C	-1.369528	-1.374433	-2.984722
C	-0.987979	-2.484959	-3.762911
H	0.074620	-2.682127	-3.963722
C	-1.966259	-3.332768	-4.302536
H	-1.658811	-4.191902	-4.917685
C	-3.328575	-3.083812	-4.070709
H	-4.092439	-3.747675	-4.502801
C	-3.711612	-1.970940	-3.304941
H	-4.776630	-1.743948	-3.145738
C	-2.740103	-1.120395	-2.757959
H	-3.056392	-0.230862	-2.192995
C	-1.065050	0.936903	-5.437942
H	-0.531539	1.628403	-6.130010
H	-0.321811	0.145782	-5.203448
C	-2.279250	0.316463	-6.145901
H	-1.999738	-0.204473	-7.087947
H	-3.042206	1.080106	-6.402114
H	-2.788918	-0.428905	-5.501970
C	2.483920	2.328237	0.559810
C	3.393146	3.164383	1.244136
H	3.832114	2.835529	2.199272
C	3.724273	4.419534	0.716697
H	4.434940	5.066804	1.253362
C	3.144111	4.856520	-0.488367
H	3.398690	5.848477	-0.892098
C	2.237080	4.033366	-1.170676
H	1.755417	4.360566	-2.105122
C	1.915029	2.770211	-0.647986
H	1.208422	2.129168	-1.189456
C	1.755884	1.054497	2.998745
C	2.328944	0.299312	4.042764
H	2.996855	-0.544388	3.818462
C	2.052388	0.617943	5.381056
H	2.509817	0.022197	6.184807
C	1.192575	1.681705	5.693271
H	0.979189	1.929680	6.744185
C	0.606295	2.428786	4.657592
H	-0.066000	3.268620	4.892408
C	0.885611	2.120022	3.320065
H	0.436580	2.720966	2.514021
C	3.656141	-0.253147	1.206617
H	4.362892	0.255557	1.895862
H	3.424374	-1.260739	1.610635
C	4.215297	-0.371114	-0.210067
H	5.164425	-0.943704	-0.205483
H	4.417923	0.622884	-0.656694
H	3.502630	-0.904532	-0.867520

Conformation 3.
Multiplicity: 5
Charge: 0
E(B97-3c) = -5596.388285026355 Hartree
E(M06/def2-TZVP) = -5596.636453081783 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -5594.600260659020 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -5594.996489040624 Hartree
E(PBEh-3c) = -5589.625217250199 Hartree
E(PM6) = -2.23795 Kcal/mol
E(PM7) = 106.40593 Kcal/mol
E(ωB97X-V/def2-TZVP) = -5597.234034402487 Hartree
E(GFN1-xTB) = -152.461881746984 Hartree
E(GFN2-xTB) = -152.113314569061 Hartree
E(GFN-FF) = -19.124607277134 Hartree

Coordinates:

Cr	0.705972	0.132565	0.595169
Al	-4.014180	2.106421	-0.092685
Cl	1.582480	-0.778067	2.518205
Cl	-4.745132	2.057315	1.945252
Cl	-3.916572	4.211337	-0.695184
N	2.289055	1.391709	-1.761653
H	2.930406	1.842610	-2.419709
N	0.064033	1.327230	-0.986988
N	-2.111295	1.526783	-0.023656
P	2.805195	0.924069	-0.176599
P	-1.369561	0.897108	1.403174
P	0.547016	-2.061510	-0.550634
C	0.936624	1.640612	-1.995074
C	0.517820	2.202440	-3.207091
H	1.248584	2.417854	-3.998031
C	-0.846376	2.488924	-3.357576
H	-1.214074	2.928983	-4.296435
C	-1.737337	2.254059	-2.316779
H	-2.786837	2.556049	-2.404178
C	-1.268454	1.696095	-1.097296
C	4.215403	-0.183027	-0.492760
C	4.889032	-0.709680	0.631789
H	4.597430	-0.390139	1.644334
C	5.897052	-1.666632	0.456160
H	6.413673	-2.079640	1.335585
C	6.238831	-2.108124	-0.833839
H	7.028837	-2.862527	-0.966662
C	5.565539	-1.591298	-1.951963
H	5.826110	-1.938529	-2.963389
C	4.550980	-0.635526	-1.785012
H	3.997310	-0.260502	-2.658495
C	3.509400	2.404121	0.641244
C	4.841160	2.834343	0.471391
H	5.535318	2.249227	-0.152288
C	5.279798	4.002574	1.111621
H	6.319525	4.339958	0.982396
C	4.396743	4.738235	1.921322
H	4.748802	5.651440	2.425016
C	3.071797	4.306824	2.097665
H	2.377162	4.868709	2.740170
C	2.627800	3.138998	1.462602
H	1.594454	2.782988	1.611251
C	-2.567093	-0.294362	2.089164
C	-3.285112	-1.103799	1.185481
H	-3.147669	-0.975335	0.102019
C	-4.205578	-2.042256	1.664807
H	-4.775559	-2.655220	0.951450
C	-4.392229	-2.202487	3.046822
H	-5.117143	-2.939884	3.423576
C	-3.653341	-1.419383	3.947422
H	-3.801386	-1.536738	5.031696
C	-2.743308	-0.463208	3.474347
H	-2.199831	0.177062	4.183985
C	-1.119129	2.283349	2.571539
C	-0.327158	2.055079	3.720492
H	0.078103	1.050261	3.919633
C	-0.007171	3.123073	4.570895
H	0.606618	2.939559	5.465978
C	-0.450185	4.422397	4.270119
H	-0.194155	5.260367	4.936750
C	-1.212211	4.651115	3.112785
H	-1.557219	5.666685	2.866291
C	-1.550233	3.589121	2.260520
H	-2.137387	3.786761	1.350507
C	-4.932897	0.934737	-1.404373
H	-4.154231	0.444687	-2.036141
H	-5.402246	0.106147	-0.827137
C	-5.981044	1.619757	-2.293581
H	-6.457391	0.927428	-3.022966
H	-5.542881	2.460003	-2.872929
H	-6.798207	2.062400	-1.686278
C	-0.738851	-3.196662	0.111777
C	-0.804069	-3.330960	1.516672
H	-0.156784	-2.707116	2.154638
C	-1.698487	-4.243231	2.091254
H	-1.748295	-4.336077	3.186280
C	-2.549141	-5.009095	1.277778
H	-3.260587	-5.714542	1.733437
C	-2.502249	-4.860775	-0.117180
H	-3.170545	-5.454657	-0.759519
C	-1.595524	-3.963101	-0.702894
H	-1.551745	-3.863281	-1.797774
C	0.183298	-1.854489	-2.331640
C	-1.068805	-1.305307	-2.692879
H	-1.829674	-1.115500	-1.919563
C	-1.347022	-0.978114	-4.025393
H	-2.326700	-0.548199	-4.282674
C	-0.373057	-1.176373	-5.018277
H	-0.588834	-0.912561	-6.064581
C	0.878585	-1.705754	-4.667815
H	1.647080	-1.862387	-5.440478
C	1.158521	-2.042337	-3.333817
H	2.147365	-2.449675	-3.076139
C	2.088074	-3.092535	-0.420949
H	2.885672	-2.533413	-0.951396
H	2.349231	-3.020800	0.656134
C	1.983027	-4.539923	-0.893573
H	2.957989	-5.056257	-0.776496
H	1.690770	-4.608362	-1.961084
H	1.228506	-5.100209	-0.307095

Conformation 34.

Multiplicity: 5
Charge: 0
E(B97-3c) = -5596.380713574475 Hartree
E(M06/def2-TZVP) = -5596.629801015921 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -5594.593726632473 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -5594.990670524994 Hartree
E(PBEh-3c) = -5589.619190962568 Hartree
E(PM6) = -1.13712 Kcal/mol
E(PM7) = 122.68174 Kcal/mol
E(ωB97X-V/def2-TZVP) = -5597.228309406410 Hartree
E(GFN1-xTB) = -152.459079655257 Hartree
E(GFN2-xTB) = -152.107621759448 Hartree
E(GFN-FF) = -19.085915780954 Hartree

Coordinates:

Cr	0.129793	-0.417705	-0.299332
Al	-3.785280	2.863836	0.270108
Cl	0.933795	-0.628176	-2.433145
Cl	-5.381433	1.452142	0.734459
Cl	-3.525005	4.341928	1.874054
N	-0.681760	-2.515237	1.858843
H	-0.852408	-3.305417	2.486562
N	-1.272409	-0.323860	1.253338
N	-2.154539	1.740641	0.434900
P	0.050239	-2.750903	0.307031
P	-1.143342	1.457610	-0.923080
P	2.367988	-0.024861	0.854439
C	-1.354178	-1.339171	2.168332
C	-2.062479	-1.215831	3.371370
H	-2.099340	-2.056833	4.077003
C	-2.683687	0.012293	3.644301
H	-3.207532	0.161686	4.600272
C	-2.666753	1.037011	2.703179
H	-3.156575	2.002754	2.884772
C	-2.020404	0.829707	1.457176
C	1.455697	-3.832577	0.752123
C	2.042195	-3.750550	2.033464
H	1.611848	-3.082339	2.794261
C	3.188835	-4.502871	2.330303
H	3.637541	-4.431958	3.332801
C	3.764305	-5.329577	1.352096
H	4.665218	-5.916758	1.585509
C	3.187831	-5.405326	0.072748
H	3.636931	-6.049866	-0.697847
C	2.038888	-4.661306	-0.230036
H	1.591533	-4.722528	-1.234203
C	-1.071553	-3.814460	-0.679321
C	-1.704277	-3.213000	-1.786817
H	-1.445163	-2.180042	-2.072465
C	-2.648285	-3.938064	-2.530005
H	-3.140413	-3.459676	-3.390218
C	-2.958500	-5.258870	-2.172178
H	-3.700714	-5.827060	-2.753468
C	-2.320010	-5.864125	-1.074323
H	-2.561267	-6.902545	-0.800340
C	-1.375054	-5.147045	-0.328029
H	-0.868863	-5.627354	0.524699
C	-0.331732	3.033875	-1.356030
C	0.716068	2.996921	-2.303507
H	1.038107	2.030546	-2.723733
C	1.357562	4.186273	-2.676424
H	2.173178	4.154304	-3.414475
C	0.975798	5.407216	-2.097276
H	1.482404	6.338952	-2.392487
C	-0.032722	5.433899	-1.121660
H	-0.321968	6.383447	-0.646231
C	-0.684030	4.251449	-0.740248
H	-1.454035	4.286699	0.046056
C	-2.254327	0.975520	-2.299558
C	-2.001985	1.322813	-3.639736
H	-1.185924	2.017348	-3.885873
C	-2.801176	0.788616	-4.661168
H	-2.603927	1.068575	-5.707064
C	-3.848515	-0.094944	-4.354324
H	-4.475301	-0.508371	-5.159064
C	-4.106204	-0.434349	-3.015779
H	-4.942099	-1.103491	-2.761826
C	-3.310777	0.093136	-1.988719
H	-3.535089	-0.160119	-0.941576
C	-3.978358	3.752862	-1.495381
H	-4.128732	4.825030	-1.231117
H	-3.026549	3.731971	-2.067795
C	-5.133454	3.261695	-2.379842
H	-5.271741	3.894228	-3.284305
H	-6.097822	3.253484	-1.831007
H	-4.964546	2.223701	-2.731083
C	2.938748	1.691814	0.500435
C	2.194420	2.766557	1.034192
H	1.312782	2.575778	1.665541
C	2.563557	4.089570	0.766323
H	1.969464	4.912388	1.189570
C	3.667147	4.361418	-0.058699
H	3.946521	5.402306	-0.280360
C	4.397307	3.300598	-0.612231
H	5.257129	3.503805	-1.268848
C	4.037442	1.971318	-0.336475
H	4.625839	1.156316	-0.780687
C	2.370466	-0.075489	2.703600
C	1.214400	0.349993	3.391299
H	0.338193	0.703100	2.830244
C	1.160806	0.312032	4.792776
H	0.246869	0.646985	5.305948
C	2.256787	-0.163314	5.527589
H	2.213412	-0.199065	6.626764
C	3.412857	-0.590047	4.852851
H	4.281262	-0.955362	5.422552
C	3.473030	-0.543566	3.452214
H	4.391648	-0.872794	2.946900
C	3.825493	-1.098137	0.408356
H	4.743702	-0.553889	0.717481
H	3.743227	-1.986810	1.065479
C	3.911036	-1.538834	-1.052716
H	4.836938	-2.128456	-1.210743
H	3.909394	-0.685277	-1.757136
H	3.046608	-2.167944	-1.334324

Conformation 4.
Multiplicity: 5
Charge: 0
E(B97-3c) = -5596.393395311546 Hartree
E(M06/def2-TZVP) = -5596.640177094025 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -5594.605472482395 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -5595.002097578518 Hartree
E(PBEh-3c) = -5589.631420967067 Hartree
E(PM6) = -8.32198 Kcal/mol
E(PM7) = 104.41180 Kcal/mol
E(ωB97X-V/def2-TZVP) = -5597.239390152394 Hartree
E(GFN1-xTB) = -152.465031779568 Hartree
E(GFN2-xTB) = -152.114128355145 Hartree
E(GFN-FF) = -19.127906897701 Hartree

Coordinates:

Cr	0.851843	-0.149373	-0.042183
Al	-3.885964	-1.774537	1.024903
Cl	2.164236	-0.764231	-1.829198
Cl	-4.080215	-2.717974	2.999136
Cl	-4.959790	0.140992	0.959741
N	1.860850	0.980238	2.673361
H	2.341399	1.266018	3.530539
N	-0.115799	0.036732	1.795297
N	-2.007867	-1.157183	0.963230
P	2.725289	0.339480	1.321347
P	-0.937174	-1.658414	-0.293193
P	0.222623	2.069408	-0.963426
C	0.501599	0.700581	2.821779
C	-0.174235	1.085337	3.985224
H	0.355450	1.634620	4.775190
C	-1.528137	0.740354	4.098419
H	-2.095532	1.031783	4.994738
C	-2.157537	0.007009	3.099648
H	-3.199199	-0.310439	3.212984
C	-1.431623	-0.374869	1.942778
C	3.915021	1.654492	0.905656
C	3.852386	2.939148	1.482636
H	3.113307	3.150376	2.269833
C	4.706590	3.955245	1.026080
H	4.655916	4.955711	1.482051
C	5.614564	3.699281	-0.013445
H	6.278046	4.499428	-0.374682
C	5.669857	2.421970	-0.597645
H	6.371452	2.221911	-1.421447
C	4.824335	1.400608	-0.145016
H	4.842573	0.409871	-0.625320
C	3.735047	-1.066958	1.918738
C	3.169578	-2.350054	1.762197
H	2.194479	-2.457054	1.257466
C	3.853924	-3.478983	2.232490
H	3.405862	-4.475896	2.103173
C	5.106209	-3.330528	2.851094
H	5.647669	-4.216837	3.215641
C	5.677036	-2.054197	2.997800
H	6.662475	-1.942990	3.475389
C	4.996232	-0.920234	2.531010
H	5.448380	0.079121	2.631680
C	-1.927493	-1.646859	-1.824788
C	-2.877307	-0.622078	-2.017015
H	-3.075610	0.114492	-1.225340
C	-3.623880	-0.573765	-3.200406
H	-4.378276	0.215850	-3.326719
C	-3.409471	-1.524135	-4.210942
H	-3.997187	-1.483101	-5.140564
C	-2.445834	-2.528919	-4.031844

H	-2.277194	-3.280502	-4.817954
C	-1.707026	-2.595856	-2.841428
H	-0.974614	-3.403302	-2.695465
C	-0.444034	-3.389649	0.058823
C	0.668593	-3.920845	-0.633533
H	1.192643	-3.305058	-1.383052
C	1.132743	-5.208042	-0.324981
H	1.997341	-5.618791	-0.868724
C	0.508058	-5.960706	0.684504
H	0.877141	-6.968743	0.928638
C	-0.580040	-5.420543	1.388938
H	-1.065651	-5.999574	2.189021
C	-1.059229	-4.137247	1.083809
H	-1.899328	-3.718297	1.660732
C	-4.376475	-3.111624	-0.352043
H	-4.604370	-2.595893	-1.308771
H	-3.493964	-3.753793	-0.572477
C	-5.563813	-3.992574	0.070350
H	-5.814702	-4.761563	-0.693241
H	-6.482067	-3.389334	0.234964
H	-5.361642	-4.521362	1.024645
C	-0.827882	2.041125	-2.472425
C	-0.448574	1.147655	-3.498609
H	0.389485	0.451036	-3.332442
C	-1.147348	1.140423	-4.713011
H	-0.850331	0.436629	-5.504826
C	-2.238601	2.002558	-4.906924
H	-2.794040	1.984526	-5.857021
C	-2.631127	2.875353	-3.880032
H	-3.490403	3.548183	-4.024319
C	-1.925719	2.902584	-2.666756
H	-2.228728	3.598082	-1.870029
C	-0.688830	3.054402	0.279541
C	-0.095941	4.125885	0.980870
H	0.908303	4.482779	0.707310
C	-0.781852	4.743285	2.039057
H	-0.310932	5.581439	2.575751
C	-2.060337	4.298970	2.412145
H	-2.592648	4.784206	3.244280
C	-2.653466	3.226965	1.725209
H	-3.644236	2.842193	2.009876
C	-1.970446	2.605530	0.672607
H	-2.445121	1.747272	0.172393
C	1.673233	3.091149	-1.517928
H	2.283412	3.281247	-0.611397
H	2.269796	2.380705	-2.128452
C	1.353274	4.374461	-2.279967
H	2.288427	4.909599	-2.544476
H	0.725447	5.065632	-1.682093
H	0.806716	4.158980	-3.219161

Conformation 8.
Multiplicity: 5
Charge: 0
E(B97-3c) = -5596.388164410458 Hartree
E(M06/def2-TZVP) = -5596.635454850569 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -5594.600298670206 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -5594.997220541527 Hartree
E(PBEh-3c) = -5589.625248199500 Hartree
E(PM6) = -6.60257 Kcal/mol
E(PM7) = 97.36029 Kcal/mol
E(ωB97X-V/def2-TZVP) = -5597.234767327922 Hartree
E(GFN1-xTB) = -152.464141699474 Hartree
E(GFN2-xTB) = -152.113454681391 Hartree
E(GFN-FF) = -19.126872343514 Hartree

Coordinates:

Cr	0.123190	0.706834	0.515218
Al	0.588363	-4.396157	0.869767
Cl	1.872643	2.185773	0.360448
Cl	-0.296884	-4.782115	2.826314
Cl	-0.484770	-5.444816	-0.747886
N	-2.561846	1.133173	2.034900
H	-3.329178	1.365636	2.671603
N	-1.309315	-0.663051	1.152324
N	0.100253	-2.500364	0.560734
P	-1.120322	2.091672	1.982486
P	1.319032	-1.315020	0.298436
P	-0.969271	1.025835	-1.720486
C	-2.493836	-0.218117	1.675240
C	-3.599314	-1.056777	1.850922
H	-4.534176	-0.658322	2.267934
C	-3.476243	-2.396458	1.449493
H	-4.339377	-3.073743	1.528337
C	-2.267259	-2.881104	0.966562
H	-2.155508	-3.923601	0.645429
C	-1.150562	-2.012045	0.876780
C	-1.698563	3.757594	1.523453
C	-0.699507	4.721022	1.259306
H	0.363021	4.445443	1.356038
C	-1.065550	6.003445	0.829146
H	-0.284501	6.749312	0.617919
C	-2.420746	6.332378	0.653782
H	-2.703491	7.339414	0.311829
C	-3.413199	5.372328	0.905498
H	-4.474942	5.623874	0.761679
C	-3.055656	4.085053	1.336018
H	-3.835531	3.327467	1.504317
C	-0.504586	2.250409	3.699739
C	-0.986445	3.209863	4.612971
H	-1.740837	3.946192	4.293389
C	-0.490514	3.229856	5.924772
H	-0.864162	3.978533	6.639855
C	0.487115	2.302173	6.324152
H	0.876651	2.326394	7.353305
C	0.976444	1.353345	5.411353
H	1.752416	0.633650	5.713342
C	0.485712	1.328315	4.099101
H	0.878121	0.599642	3.369269
C	2.045361	-1.604276	-1.350956
C	1.701389	-2.722554	-2.136700
H	1.018901	-3.495179	-1.749540
C	2.224268	-2.848395	-3.431947
H	1.951606	-3.724721	-4.039238
C	3.088724	-1.869499	-3.946395
H	3.492877	-1.970626	-4.965056
C	3.424375	-0.751376	-3.166667
H	4.078907	0.032091	-3.575762
C	2.895580	-0.606402	-1.876524
H	3.105517	0.300520	-1.286776
C	2.604353	-1.629725	1.560474
C	2.162093	-1.908921	2.872745
H	1.089383	-2.049971	3.077173
C	3.095556	-2.074679	3.904080
H	2.744483	-2.323639	4.917129
C	4.470157	-1.948855	3.639917
H	5.202409	-2.083036	4.450418
C	4.908179	-1.665643	2.336823
H	5.984203	-1.578467	2.123044
C	3.980690	-1.503745	1.296347
H	4.331610	-1.298335	0.274385
C	2.497166	-4.905944	0.919731
H	2.972617	-4.400428	1.787983
H	2.380643	-5.966156	1.251367
C	3.421012	-4.863424	-0.301196
H	4.381291	-5.395621	-0.122645
H	3.682878	-3.824751	-0.588249
H	2.950509	-5.331028	-1.191507
C	0.110244	1.165780	-3.202847
C	1.182954	2.080875	-3.114966
H	1.384480	2.594410	-2.160616
C	2.012302	2.299621	-4.223631
H	2.843816	3.016901	-4.145799
C	1.799504	1.591740	-5.417759
H	2.458750	1.756112	-6.283790
C	0.747341	0.666720	-5.500357
H	0.577251	0.104642	-6.431358
C	-0.102414	0.459074	-4.402829
H	-0.935599	-0.254025	-4.482813
C	-2.148218	-0.337347	-2.053274
C	-3.537136	-0.190543	-1.852023
H	-3.962898	0.789998	-1.593650
C	-4.390116	-1.299247	-1.966309
H	-5.471445	-1.169279	-1.806409
C	-3.870205	-2.566435	-2.270243
H	-4.540354	-3.436062	-2.344565
C	-2.487564	-2.726149	-2.454682
H	-2.058513	-3.722551	-2.636493
C	-1.634090	-1.621146	-2.344342
H	-0.550316	-1.764304	-2.460853
C	-1.963292	2.598154	-1.823988
H	-2.710059	2.544717	-1.004560
H	-1.250163	3.389778	-1.511290
C	-2.598467	2.918549	-3.174667
H	-3.156352	3.876108	-3.123129
H	-3.306067	2.128618	-3.496055
H	-1.826980	3.015140	-3.963948

UZEYAA

Conformation 14.
Multiplicity: 3
Charge: 0
E(B97-3c) = -3893.561204159994 Hartree
E(M06/def2-TZVP) = -3893.294578076202 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3891.975745389707 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3892.237337119500 Hartree
E(PBEh-3c) = -3888.291926142691 Hartree
E(PM6) = 88.99137 Kcal/mol
E(PM7) = 41.77057 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3895.850580102099 Hartree

E(GFN1-xTB) = -161.271244584265 Hartree
E(GFN2-xTB) = -160.183795911328 Hartree
E(GFN-FF) = -22.397406714193 Hartree

Coordinates:

Co	-0.172086	-0.355137	-0.146222
N	1.456171	0.791283	-0.325789
N	-1.116257	0.306368	-1.709477
C	3.008065	2.311970	-1.773283
C	1.659692	1.578250	-1.395316
C	0.658924	1.768220	-2.381168
H	0.950545	2.465317	-3.166786
C	-0.648684	1.261874	-2.536877
C	-1.435931	1.934978	-3.721952
C	3.529501	1.635803	-3.068340
H	4.478689	2.113246	-3.388851
H	2.805356	1.708164	-3.901512
H	3.732636	0.559654	-2.896171
C	2.747324	3.812706	-2.056495
H	3.703940	4.307556	-2.321877
H	2.343030	4.324680	-1.159890
H	2.043950	3.988571	-2.891998
C	4.171129	2.275143	-0.761506
H	5.047609	2.759497	-1.239794
H	4.472670	1.254091	-0.476320
H	3.954404	2.829669	0.168250
C	-0.577866	1.895495	-5.014534
H	-1.162781	2.320713	-5.855480
H	-0.301085	0.857109	-5.282098
H	0.355928	2.483684	-4.939513
C	-2.798159	1.323355	-4.108763
H	-3.183384	1.876833	-4.989614
H	-3.556057	1.400715	-3.311390
H	-2.721542	0.257698	-4.391275
C	-1.680168	3.414527	-3.334319
H	-2.219043	3.939857	-4.150562
H	-0.730033	3.950700	-3.145084
H	-2.295720	3.491414	-2.417065
C	2.329780	0.733371	0.785760
C	3.182309	-0.387033	1.005607
C	3.999506	-0.382470	2.156430
H	4.645038	-1.255786	2.343202
C	4.031331	0.700322	3.040993
H	4.696379	0.681996	3.917343
C	3.196747	1.803749	2.806234
H	3.215304	2.651760	3.504811
C	2.321054	1.831390	1.710609
C	3.383554	-1.579328	0.058045
H	3.392207	-2.469461	0.724277
C	2.319985	-1.848357	-1.008978
H	1.304528	-1.874004	-0.555576
H	2.487907	-2.845724	-1.464396
H	2.320580	-1.094320	-1.817286
C	4.770392	-1.520469	-0.617138
H	4.967134	-2.457704	-1.177385
H	5.585328	-1.383478	0.120339
H	4.824817	-0.681408	-1.339620
C	1.383818	3.013068	1.476091
H	1.405824	3.232636	0.388773
C	-0.071627	2.644101	1.807343
H	-0.357632	1.704679	1.293011
H	-0.766910	3.442214	1.476091
H	-0.212598	2.483261	2.894493
C	1.799234	4.296247	2.202392
H	1.140766	5.135058	1.898587
H	2.845465	4.583912	1.971535
H	1.708230	4.195915	3.304213
C	-2.423759	-0.248314	-1.750613
C	-3.490978	0.423753	-1.074408
C	-4.785132	-0.122078	-1.116496
H	-5.604989	0.398715	-0.598655
C	-5.049467	-1.310945	-1.807113
H	-6.071361	-1.717310	-1.849142
C	-3.992710	-1.986726	-2.428227
H	-4.185388	-2.939458	-2.947435
C	-2.674686	-1.491780	-2.410663
C	-3.238094	1.682342	-0.253475
H	-2.235947	2.064570	-0.534048
C	-4.262279	2.796408	-0.515304
H	-4.355346	3.023375	-1.596248
H	-3.959846	3.727799	0.005608
H	-5.271842	2.526958	-0.141934
C	-3.185725	1.311588	1.237640
H	-2.370043	0.585864	1.425560
H	-4.135582	0.840646	1.565059
H	-2.996059	2.198437	1.874588
C	-1.596805	-2.399931	-3.004499
H	-2.146261	-3.112637	-3.657550
C	-0.512748	-1.756738	-3.880214
H	-0.952001	-1.125365	-4.677277
H	0.079474	-2.553582	-4.375372
H	0.185143	-1.129436	-3.294870
C	-0.969613	-3.221780	-1.867653
H	-1.725942	-3.827786	-1.331798
H	-0.522305	-2.522959	-1.125472
H	-0.164457	-3.890101	-2.236479
P	-0.320275	-1.543158	1.769640
C	0.928347	-2.881029	2.127351
C	1.001858	-3.933327	1.187153
H	0.311895	-3.951087	0.331452
C	1.935903	-4.966107	1.336062
H	1.974861	-5.774196	0.589934
C	2.817238	-4.969073	2.430255
H	3.557192	-5.775518	2.544208
C	2.732604	-3.944576	3.384223
H	3.401690	-3.946408	4.258448
C	1.792626	-2.910797	3.238433
H	1.733841	-2.129587	4.007128
C	-1.853974	-2.587397	1.921216
C	-2.946888	-2.397642	1.058984
H	-2.889367	-1.649480	0.257651
C	-4.119196	-3.156555	1.218374
H	-4.960042	-2.991349	0.529042
C	-4.207065	-4.109934	2.241999
H	-5.126096	-4.702315	2.369595
C	-3.116813	-4.306359	3.107958
H	-3.179140	-5.052765	3.914520
C	-1.946942	-3.553149	2.948017
H	-1.095753	-3.711525	3.627589
C	-0.437726	-0.584885	3.347862
C	-1.687450	-0.334924	3.955383
H	-2.598479	-0.794661	3.546460
C	-1.776473	0.499217	5.079974
H	-2.759855	0.688770	5.537243
C	-0.621010	1.080622	5.627177
H	-0.692652	1.729400	6.513423
C	0.624345	0.834091	5.029944
H	1.540338	1.289572	5.435309
C	0.713055	0.022217	3.890265
H	1.687599	-0.124273	3.411380

Conformation 19.
Multiplicity: 3
Charge: 0
E(B97-3c) = -3893.559999889183 Hartree
E(M06/def2-TZVP) = -3893.292016440676 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3891.974521353261 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3892.235869461007 Hartree
E(PBEh-3c) = -3888.292285114661 Hartree
E(PM6) = 88.38083 Kcal/mol
E(PM7) = 51.12475 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3895.849692308639 Hartree
E(GFN1-xTB) = -161.269486258523 Hartree
E(GFN2-xTB) = -160.182943194542 Hartree
E(GFN-FF) = -22.395905907788 Hartree

Coordinates:

Co	0.072310	-0.206940	0.235800
N	-0.988378	1.414448	0.617536
N	1.791638	0.666641	0.001662
C	-1.223241	4.002259	0.800963
C	-0.437344	2.635647	0.756076
C	0.972101	2.802596	0.752072
H	1.299783	3.809061	1.013280
C	2.026508	1.942003	0.389678
C	3.455242	2.581559	0.570517
C	-0.562125	5.018420	1.769189
H	-1.203344	5.920191	1.833875
H	0.433672	5.365586	1.433514
H	-0.457936	4.607175	2.791754
C	-1.133660	4.594498	-0.630191
H	-1.630234	5.586859	-0.663194
H	-1.635261	3.942097	-1.370708
H	-0.078997	4.719508	-0.946250
C	-2.710922	3.947785	1.205164
H	-3.097840	4.986951	1.239547
H	-2.862572	3.500665	2.203658
H	-3.338823	3.387046	0.495278
C	3.626823	2.826205	2.093739
H	4.619038	3.280711	2.296755
H	3.568797	1.873378	2.656783
H	2.847444	3.500570	2.497204
C	4.657997	1.733066	0.112040
H	5.586480	2.257266	0.419265
H	4.695737	1.598182	-0.983518
H	4.674504	0.732324	0.573474
C	3.567387	3.939169	-0.163402
H	4.572414	4.373724	0.014887
H	2.822287	4.682504	0.179276
H	3.447053	3.818791	-1.258287
C	-2.339283	1.102463	0.911622
C	-2.698211	0.765103	2.253296

C	-4.052651	0.497484	2.532516	Conformation 20.
H	-4.335280	0.252373	3.569383	Multiplicity: 3
C	-5.037171	0.543732	1.536610	Charge: 0
H	-6.090152	0.343592	1.786157	E(B97-3c) = -3893.569504779442 Hartree
C	-4.661799	0.826281	0.216948	E(M06/def2-TZVP) = -3893.298385363765 Hartree
H	-5.428228	0.841967	-0.572396	E(PBE - D3(BJ)/def2-TZVP) = -3891.984093131889 Hartree
C	-3.326811	1.102416	-0.120003	E(PBE0 - D3(BJ)/def2-TZVP) = -3892.245171708628 Hartree
C	-1.711096	0.699771	3.422856	E(PBEh-3c) = -3888.303727951105 Hartree
H	-2.277874	0.187423	4.231020	E(PM6) = 80.46644 Kcal/mol
C	-0.473401	-0.170009	3.168296	E(PM7) = 36.81475 Kcal/mol
H	-0.773426	-1.175459	2.828043	E(ωB97X-V/def2-TZVP) = -3895.860776698953 Hartree
H	0.113701	-0.294931	4.102066	E(GFN1-xTB) = -161.275614469677 Hartree
H	0.216194	0.286209	2.419129	E(GFN2-xTB) = -160.190050598074 Hartree
C	-1.303994	2.071020	3.987528	E(GFN-FF) = -22.406342276997 Hartree
H	-0.752177	1.939153	4.941341	
H	-2.184377	2.712533	4.190405	Coordinates:
H	-0.631898	2.605704	3.289482	Co -0.073153 -0.090218 -0.207773
C	-2.948549	1.449198	-1.555189	N -0.032710 0.890436 1.500949
H	-1.970486	1.967408	-1.502365	N -1.710473 -1.076021 0.050916
C	-2.727622	0.185356	-2.398487	C -1.011671 1.363790 3.881555
H	-1.927052	-0.432321	-1.949872	C -1.009156 0.754402 2.422490
H	-2.425011	0.446838	-3.433216	C -2.153635 -0.047294 2.174220
H	-3.643087	-0.438932	-2.445372	H -2.895061 -0.005188 2.971909
C	-3.945996	2.398284	-2.235140	C -2.522971 -0.899450 1.114239
H	-3.550909	2.730997	-3.216947	C -3.967930 -1.505945 1.263680
H	-4.140908	3.301240	-1.621984	C -2.405510 1.952481 4.232218
H	-4.920854	1.905062	-2.428858	H -2.351482 2.439974 5.226474
C	2.629897	-0.022689	-0.914115	H -3.207829 1.193333 4.295527
C	3.261841	-1.250040	-0.547923	H -2.718972 2.719947 3.497600
C	4.129259	-1.862478	-1.467633	C -0.722858 0.191622 4.853128
H	4.639566	-2.794361	-1.188671	H -0.743069 0.552977 5.902729
C	4.350670	-1.318803	-2.738404	H 0.275116 -0.249122 4.666120
H	5.040274	-1.813067	-3.439218	H -1.473576 -0.616050 4.748995
C	3.662725	-0.161226	-3.122870	C -0.008017 2.494865 4.190880
H	3.813600	0.241474	-4.134636	H -0.195040 2.840295 5.228368
C	2.792356	0.499589	-2.238032	H -0.131884 3.365485 3.522207
C	2.963579	-1.901166	0.796799	H 1.045276 2.177740 4.133953
H	1.855581	-1.789636	0.903283	C -4.961029 -0.313481 1.243138
C	3.303658	-3.392837	0.846708	H -6.001034 -0.685437 1.352807
H	2.866891	-3.946569	-0.006101	H -4.898783 0.238497 0.284530
H	2.914682	-3.846225	1.780002	H -4.764792 0.408930 2.058021
H	4.401726	-3.556461	0.841324	C -4.421828 -2.485696 0.164189
C	3.579364	-1.178129	2.005290	H -5.486333 -2.739831 0.346488
H	3.243133	-0.127374	2.063312	H -3.847022 -3.428668 0.165762
H	4.687991	-1.191703	1.957616	H -4.352164 -2.054013 -0.848911
H	3.279989	-1.681634	2.948724	C -4.118773 -2.244735 2.615242
C	2.009384	1.730902	-2.689733	H -5.150518 -2.642063 2.706333
H	2.003718	2.450758	-1.847369	H -3.938845 -1.587721 3.487854
C	2.618560	2.458145	-3.892871	H -3.423316 -3.104665 2.690641
H	3.685092	2.710497	-3.723405	C 1.088287 1.747820 1.650857
H	2.070968	3.403312	-4.083455	C 1.030236 3.072722 1.115127
H	2.556770	1.855681	-4.823086	C 2.099078 3.949055 1.376373
C	0.536687	1.376704	-2.948935	H 2.053499 4.980950 1.000233
H	0.065261	0.970751	-2.031116	C 3.226058 3.533817 2.100194
H	0.437243	0.623504	-3.757797	H 4.043817 4.241016 2.306186
H	-0.043480	2.275697	-3.242498	C 3.320101 2.201573 2.518948
P	-0.819367	-2.295139	0.026847	H 4.226981 1.860627 3.040201
C	-0.771255	-3.515786	1.437677	C 2.271579 1.290365 2.302121
C	-1.672987	-4.599593	1.514330	C -0.147535 3.503994 0.247392
H	-2.447547	-4.720376	0.743448	H -0.383640 2.602589 -0.365575
C	-1.590090	-5.526150	2.565105	C -1.417361 3.851819 1.042125
H	-2.302356	-6.364444	2.606654	H -1.767661 2.998598 1.649492
C	-0.606682	-5.387388	3.556910	H -2.239540 4.127918 0.349759
H	-0.545002	-6.113409	4.381824	H -1.240172 4.715714 1.716488
C	0.293935	-4.313361	3.491608	C 0.197105 4.650697 -0.709900
H	1.066822	-4.189574	4.265691	H -0.639502 4.823036 -1.415013
C	0.209256	-3.386190	2.442789	H 1.102167 4.435417 -1.311470
H	0.912629	-2.543884	2.410533	H 0.361796 5.603016 -0.163608
C	0.222019	-3.147810	-1.246983	C 2.408867 -0.155035 2.764218
C	0.665264	-2.377075	-2.340560	H 1.384304 -0.574047 2.823080
H	0.438079	-1.301862	-2.368871	C 3.175470 -0.980451 1.717291
C	1.398471	-2.967069	-3.378849	H 2.642564 -0.972160 0.747719
H	1.744764	-2.346218	-4.217672	H 3.282848 -2.035509 2.042651
C	1.710723	-4.334394	-3.326662	H 4.187185 -0.562938 1.537768
H	2.297412	-4.798105	-4.134302	C 3.055122 -0.295170 4.150518
C	1.281059	-5.107626	-2.235954	H 3.001397 -1.348192 4.495123
H	1.527657	-6.179454	-2.188059	H 2.552681 0.339648 4.907859
C	0.535707	-4.520648	-1.201079	H 4.128337 -0.014603 4.134882
H	0.199387	-5.132950	-0.351597	C -1.737507 -2.202812 -0.809925
C	-2.516700	-2.650447	-0.623430	C -1.397119 -3.491570 -0.287093
C	-2.745878	-3.274597	-1.865924	C -1.475832 -4.606480 -1.139509
H	-1.896520	-3.584275	-2.491570	H -1.241794 -5.605941 -0.746166
C	-4.057787	-3.500322	-2.311114	C -1.859829 -4.470775 -2.480668
H	-4.224994	-3.985755	-3.284963	H -1.935177 -5.358065 -3.127239
C	-5.150452	-3.115456	-1.518055	C -2.104635 -3.195459 -3.003901
H	-6.178492	-3.295859	-1.867613	H -2.348874 -3.090541 -4.070155
C	-4.924270	-2.495243	-0.278585	C -2.025132 -2.046391 -2.200066
H	-5.770873	-2.177265	0.348015	C -0.929457 -3.631680 1.159241
C	-3.616510	-2.254665	0.163302	H -1.608889 -3.022235 1.789268
H	-3.450541	-1.750126	1.127610	C -0.974629 -5.062308 1.703668
				H -1.980540 -5.515630 1.591836

H	-0.717117	-5.066987	2.781932
H	-0.245225	-5.724189	1.191998
C	0.471607	-3.024998	1.335302
H	0.467759	-1.953187	1.040006
H	1.225719	-3.555335	0.718590
H	0.799235	-3.063973	2.393758
C	-2.182790	-0.654946	-2.796929
H	-1.384435	-0.062586	-2.284913
C	-1.917578	-0.597419	-4.303401
H	-0.970743	-1.102149	-4.573859
H	-1.847588	0.457115	-4.638897
H	-2.740953	-1.068781	-4.880263
C	-3.516476	0.026740	-2.456126
H	-3.658593	0.114875	-1.363568
H	-4.373275	-0.540022	-2.876391
H	-3.547673	1.050271	-2.885357
P	1.486500	0.403082	-1.729798
C	1.475730	-0.984483	-2.962297
C	1.268472	-2.291580	-2.477267
H	1.053924	-2.447265	-1.409296
C	1.321745	-3.391564	-3.345348
H	1.148810	-4.402189	-2.948275
C	1.565338	-3.193790	-4.713101
H	1.595341	-4.054276	-5.398815
C	1.762810	-1.893321	-5.206216
H	1.949489	-1.732467	-6.279156
C	1.724430	-0.792925	-4.336256
H	1.883204	0.221949	-4.729547
C	3.306292	0.510152	-1.386435
C	4.194057	-0.537491	-1.707786
H	3.827180	-1.427944	-2.238123
C	5.549325	-0.452492	-1.353244
H	6.229624	-1.279442	-1.608856
C	6.037669	0.681233	-0.685065
H	7.101619	0.747172	-0.410715
C	5.158460	1.728872	-0.367102
H	5.521455	2.620410	0.166157
C	3.801508	1.641165	-0.705439
H	3.120737	2.459349	-0.429408
C	1.220801	1.878533	-2.825135
C	-0.101948	2.299143	-3.071126
H	-0.934779	1.790773	-2.563535
C	-0.366910	3.361548	-3.945961
H	-1.407479	3.671576	-4.127066
C	0.691771	4.037441	-4.572942
H	0.486855	4.879352	-5.251484
C	2.013865	3.637954	-4.322757
H	2.850685	4.164546	-4.806807
C	2.278545	2.561514	-3.460878
H	3.317395	2.249461	-3.279617

Conformation 22.
Multiplicity: 3
Charge: 0
E(B97-3c) = -3893.560355371872 Hartree
E(M06/def2-TZVP) = -3893.289586107422 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3891.975409048667 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3892.235198999790 Hartree
E(PBEh-3c) = -3888.287746335652 Hartree
E(PM6) = 89.32346 Kcal/mol
E(PM7) = 46.70307 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3895.848380704743 Hartree
E(GFN1-xTB) = -161.274026535109 Hartree
E(GFN2-xTB) = -160.183986600368 Hartree
E(GFN-FF) = -22.395614900441 Hartree

Coordinates:

Co	0.231587	-0.151408	0.155394
N	-0.845371	1.502766	0.250229
N	1.833264	0.658761	-0.574761
C	-1.094032	4.093513	0.238618
C	-0.335625	2.726165	0.050867
C	1.009140	2.903777	-0.378422
H	1.308200	3.948929	-0.477163
C	2.030629	1.988090	-0.698480
C	3.407923	2.660817	-1.057056
C	-0.251219	5.031763	1.141437
H	-0.815024	5.967866	1.331893
H	0.718826	5.318028	0.694083
H	-0.040489	4.556999	2.121016
C	-1.246340	4.733318	-1.163603
H	-1.748247	5.720024	-1.080548
H	-1.864512	4.092949	-1.824013
H	-0.269209	4.884923	-1.661854
C	-2.496450	4.049283	0.876377
H	-2.862989	5.092646	0.967261
H	-2.494362	3.605218	1.887234
H	-3.230403	3.490264	0.274375
C	3.894139	3.398706	0.218849
H	4.868621	3.891810	0.020313
H	4.037323	2.693045	1.060453
H	3.177992	4.174846	0.550559
C	4.537473	1.704269	-1.484346
H	5.469549	2.295508	-1.596625
H	4.336584	1.208666	-2.450944
H	4.732352	0.914406	-0.738747
C	3.245053	3.705393	-2.186678
H	4.222191	4.191801	-2.384710
H	2.522547	4.504054	-1.931859
H	2.910270	3.234736	-3.132414
C	-2.108773	1.217564	0.817374
C	-2.216485	0.982520	2.217242
C	-3.491398	0.688104	2.741042
H	-3.586736	0.492791	3.821528
C	-4.630607	0.632764	1.933698
H	-5.611178	0.402976	2.374907
C	-4.500989	0.827044	0.551765
H	-5.391850	0.754869	-0.091189
C	-3.254972	1.102053	-0.028796
C	-1.072843	1.060359	3.241184
H	-1.248117	0.184327	3.908531
C	0.380425	0.944011	2.757737
H	0.543087	0.027567	2.132787
H	1.051102	0.816463	3.633839
H	0.734955	1.826980	2.195800
C	-1.207845	2.313446	4.130764
H	-0.480155	2.282397	4.968010
H	-2.224773	2.402166	4.560261
H	-1.008789	3.234977	3.547824
C	-3.128412	1.284824	-1.538654
H	-2.145756	1.762926	-1.724045
C	-3.107346	-0.072980	-2.260810
H	-2.299560	-0.721589	-1.868641
H	-2.936173	0.056972	-3.348731
H	-4.073773	-0.603700	-2.130770
C	-4.212139	2.195232	-2.136476
H	-4.009987	2.383199	-3.211002
H	-4.257571	3.175888	-1.622173
H	-5.220009	1.735406	-2.070773
C	2.520778	-0.351067	-1.286972
C	3.214891	-1.387309	-0.583773
C	3.847576	-2.395381	-1.331863
H	4.392493	-3.191923	-0.807926
C	3.800527	-2.413241	-2.731975
H	4.311288	-3.210678	-3.292288
C	3.082332	-1.421107	-3.411443
H	3.029680	-1.451866	-4.509174
C	2.425169	-0.390552	-2.717644
C	3.213911	-1.427703	0.942895
H	2.136951	-1.329600	1.226745
C	3.723608	-2.747697	1.523949
H	3.177640	-3.620754	1.118240
H	3.589112	-2.754153	2.622613
H	4.806468	-2.887988	1.322444
C	3.945023	-0.248554	1.602523
H	3.517036	0.718639	1.286554
H	5.026003	-0.256569	1.350734
H	3.855886	-0.314933	2.706601
C	1.585532	0.643545	-3.461877
H	1.780327	1.627629	-2.992181
C	1.935326	0.785554	-4.946929
H	3.017422	0.975248	-5.099015
H	1.374729	1.633697	-5.389275
H	1.664228	-0.119882	-5.528966
C	0.083942	0.379240	-3.273817
H	-0.188321	0.400821	-2.197519
H	-0.212242	-0.605092	-3.688895
H	-0.519538	1.164669	-3.773213
P	-0.774077	-2.112437	0.663390
C	0.192724	-3.185877	1.847956
C	0.515708	-4.527643	1.561809
H	0.240706	-4.961350	0.590017
C	1.184017	-5.320332	2.508607
H	1.427007	-6.365952	2.264677
C	1.540286	-4.788143	3.756518
H	2.061236	-5.412299	4.498203
C	1.237663	-3.448524	4.046835
H	1.521048	-3.014018	5.017766
C	0.579992	-2.652863	3.097127
H	0.361607	-1.603338	3.337545
C	-0.833107	-3.206241	-0.835007
C	0.104270	-2.940553	-1.851777
H	0.800685	-2.096016	-1.741464
C	0.164792	-3.744527	-2.999564
H	0.911233	-3.513769	-3.774170
C	-0.719925	-4.823348	-3.147279
H	-0.681992	-5.451553	-4.050462
C	-1.654360	-5.100981	-2.135107
H	-2.346779	-5.950293	-2.241782
C	-1.709016	-4.303453	-0.982064
H	-2.437233	-4.537308	-0.191824
C	-2.476993	-2.371503	1.378890

C	-3.597333	-2.298938	0.525716
H	-3.457328	-2.076965	-0.539506
C	-4.889292	-2.532501	1.016109
H	-5.746265	-2.479546	0.327192
C	-5.091092	-2.818467	2.374166
H	-6.105889	-3.000694	2.759295
C	-3.986070	-2.868762	3.236968
H	-4.127679	-3.092379	4.305586
C	-2.690489	-2.652716	2.744305
H	-1.838557	-2.731191	3.433810

Conformation 23.
Multiplicity: 3
Charge: 0
E(B97-3c) = -3893.565328902517 Hartree
E(M06/def2-TZVP) = -3893.296543162907 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3891.979858930894 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3892.242067120452 Hartree
E(PBEh-3c) = -3888.300130612013 Hartree
E(PM6) = 82.56325 Kcal/mol
E(PM7) = 41.17791 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3895.861757008122 Hartree
E(GFN1-xTB) = -161.276371334800 Hartree
E(GFN2-xTB) = -160.190617326721 Hartree
E(GFN-FF) = -22.400222107330 Hartree

Coordinates:

Co	0.238553	0.074257	-0.119211
N	-0.898731	-1.251626	0.853661
N	0.761726	-1.133172	-1.542082
C	-1.857502	-3.660229	1.222990
C	-1.023874	-2.540483	0.479085
C	-0.363194	-3.050223	-0.663371
H	-0.531714	-4.114296	-0.837000
C	0.439522	-2.435116	-1.645641
C	0.865666	-3.410455	-2.803028
C	-2.862423	-4.293041	0.225907
H	-3.448343	-5.083787	0.738157
H	-2.372141	-4.756181	-0.650730
H	-3.577627	-3.534628	-0.151436
C	-0.861786	-4.748538	1.701668
H	-1.414543	-5.572306	2.199361
H	-0.142415	-4.333148	2.436483
H	-0.275437	-5.184821	0.870978
C	-2.689930	-3.261673	2.459698
H	-3.175657	-4.181295	2.846837
H	-3.489107	-2.536109	2.228410
H	-2.083403	-2.841540	3.279727
C	-0.419175	-3.963504	-3.469691
H	-0.146668	-4.660652	-4.289086
H	-1.019726	-3.140195	-3.906433
H	-1.067867	-4.511178	-2.760555
C	1.734584	-2.845936	-3.945051
H	1.908236	-3.666278	-4.671872
H	2.723677	-2.494546	-3.603282
H	1.254822	-2.015042	-4.491262
C	1.675299	-4.579423	-2.187484
H	1.974384	-5.289866	-2.985964
H	1.104905	-5.147824	-1.428128
H	2.600453	-4.203482	-1.705026
C	-1.656081	-0.660338	1.894057
C	-2.979563	-0.197389	1.622149
C	-3.716151	0.385235	2.667386
H	-4.743669	0.726892	2.476618
C	-3.158883	0.551863	3.943880
H	-3.743276	1.031142	4.744304
C	-1.867246	0.069280	4.205646
H	-1.457935	0.150502	5.223079
C	-1.113198	-0.578508	3.211062
C	-3.578780	-0.395058	0.233326
H	-3.204178	-1.372740	-0.136363
C	-5.109795	-0.460329	0.220196
H	-5.496124	-1.220164	0.929762
H	-5.472730	-0.722555	-0.794376
H	-5.565126	0.516635	0.484702
C	-3.074630	0.662208	-0.760860
H	-3.362026	0.398108	-1.798450
H	-1.966846	0.742412	-0.721572
H	-3.478084	1.667125	-0.527035
C	0.174239	-1.329716	3.544612
H	0.168336	-2.228536	2.892048
C	1.445629	-0.551482	3.191046
H	1.391114	-0.170768	2.151954
H	2.343067	-1.197741	3.279511
H	1.577198	0.318103	3.862347
C	0.232173	-1.818696	4.997791
H	1.106113	-2.486260	5.142657
H	-0.680223	-2.380962	5.284129
H	0.349914	-0.974727	5.709084
C	1.551111	-0.413399	-2.471909
C	0.921976	0.325487	-3.515316
C	1.732131	1.015086	-4.435297
H	1.256953	1.578472	-5.253453
C	3.128438	0.999284	-4.328873
H	3.745056	1.536851	-5.065257
C	3.737385	0.311170	-3.267808
H	4.833247	0.322186	-3.176108
C	2.972689	-0.399119	-2.329362
C	-0.595251	0.400559	-3.623398
H	-1.007061	-0.247897	-2.822711
C	-1.073906	1.835575	-3.349687
H	-0.761345	2.166770	-2.340024
H	-2.178948	1.907123	-3.398834
H	-0.650900	2.552444	-4.083333
C	-1.119550	-0.122491	-4.969999
H	-0.802898	-1.169053	-5.152051
H	-0.753627	0.490626	-5.819750
H	-2.228223	-0.093163	-4.994002
C	3.619541	-1.116309	-1.152810
H	2.964935	-1.975859	-0.899187
C	5.018871	-1.668666	-1.444766
H	5.020352	-2.320337	-2.342065
H	5.381860	-2.268660	-0.586105
H	5.761658	-0.861074	-1.609994
C	3.627343	-0.182863	0.068484
H	2.597422	0.190807	0.272736
H	4.266671	0.705011	-0.117244
H	3.988275	-0.698359	0.981351
P	0.384851	2.210722	0.664842
C	-1.174761	3.210920	0.642683
C	-1.432455	4.134352	-0.394277
H	-0.667657	4.329368	-1.158819
C	-2.657352	4.814978	-0.456074
H	-2.836949	5.532586	-1.271174
C	-3.642875	4.594725	0.519582
H	-4.599679	5.136782	0.475674
C	-3.399506	3.668995	1.545309
H	-4.165400	3.463933	2.308906
C	-2.184215	2.971121	1.595494
H	-2.044354	2.210472	2.372153
C	1.489841	3.354604	-0.306649
C	1.719592	4.663006	0.178523
H	1.251118	4.984364	1.120688
C	2.536493	5.549205	-0.532326
H	2.707253	6.565048	-0.144447
C	3.138871	5.142148	-1.736844
H	3.781646	5.839925	-2.295550
C	2.917501	3.846749	-2.221257
H	3.381426	3.509389	-3.159626
C	2.095349	2.955669	-1.507426
H	1.926025	1.943434	-1.892880
C	1.143286	2.568397	2.333036
C	2.550014	2.453602	2.415705
H	3.132568	2.219824	1.512831
C	3.217208	2.643342	3.631778
H	4.313346	2.550658	3.670504
C	2.491886	2.955360	4.793725
H	3.013287	3.107704	5.750555
C	1.097360	3.079018	4.720289
H	0.516087	3.334055	5.619575
C	0.426463	2.888798	3.500415
H	-0.662965	3.007532	3.472853

Conformation 3.
Multiplicity: 3
Charge: 0
E(B97-3c) = -3893.562220761271 Hartree
E(M06/def2-TZVP) = -3893.294167850594 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3891.977074941923 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3892.238360477379 Hartree
E(PBEh-3c) = -3888.297655951989 Hartree
E(PM6) = 81.61264 Kcal/mol
E(PM7) = 38.74997 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3895.855103885208 Hartree
E(GFN1-xTB) = -161.271953209007 Hartree
E(GFN2-xTB) = -160.184795360752 Hartree
E(GFN-FF) = -22.403775828697 Hartree

Coordinates:

Co	0.051448	-0.208423	0.187197
N	-1.017070	0.937339	-1.016851
N	-1.040254	-0.025945	1.764722
C	-3.038280	2.546004	-1.452888
C	-2.177724	1.507303	-0.627000
C	-2.722249	1.271390	0.659974
H	-3.687531	1.750947	0.823237
C	-2.232547	0.597358	1.798263
C	-3.204093	0.659900	3.035353
C	-4.549232	2.194113	-1.388202
H	-5.113638	2.921549	-2.006041
H	-4.977153	2.242492	-0.369272
H	-4.749550	1.183743	-1.794420

C	-2.835304	3.924545	-0.774261
H	-3.398331	4.707666	-1.324083
H	-1.767928	4.215277	-0.765534
H	-3.188889	3.915491	0.275223
C	-2.727711	2.702056	-2.956201
H	-3.465280	3.410902	-3.385553
H	-2.819236	1.749754	-3.508174
H	-1.723864	3.107004	-3.159265
C	-4.591916	0.127742	2.590920
H	-5.288080	0.136273	3.454905
H	-4.520452	-0.915336	2.222317
H	-5.048346	0.733866	1.786161
C	-2.808649	-0.163036	4.278300
H	-3.628012	-0.074774	5.021308
H	-1.882082	0.194265	4.760175
H	-2.683553	-1.237456	4.052517
C	-3.356804	2.130934	3.491190
H	-4.087022	2.195389	4.324536
H	-3.714137	2.787737	2.674459
H	-2.394413	2.539359	3.856750
C	-0.467612	1.066270	-2.319459
C	0.392600	2.154855	-2.649746
C	0.835010	2.289996	-3.978023
H	1.483129	3.139703	-4.241575
C	0.461658	1.375602	-4.968737
H	0.795684	1.512251	-6.008452
C	-0.309301	0.258089	-4.615607
H	-0.559683	-0.485439	-5.385402
C	-0.768554	0.068015	-3.299978
C	0.831614	3.179235	-1.609382
H	0.211082	3.010496	-0.705347
C	2.301389	2.955684	-1.216142
H	2.455552	1.944233	-0.799359
H	2.627592	3.698473	-0.459492
H	2.967556	3.051294	-2.097703
C	0.621433	4.631457	-2.071499
H	0.820474	5.335304	-1.237342
H	-0.410580	4.811222	-2.431362
H	1.314222	4.899886	-2.895623
C	-1.538120	-1.190266	-2.910220
H	-1.145266	-1.448691	-1.898566
C	-3.054164	-0.984405	-2.753279
H	-3.290976	-0.251612	-1.962510
H	-3.541040	-1.941537	-2.473187
H	-3.511418	-0.639234	-3.704167
C	-1.277371	-2.367921	-3.855521
H	-1.727294	-3.293291	-3.446670
H	-0.196380	-2.555811	-4.004640
H	-1.739381	-2.195123	-4.850138
C	-0.301303	-0.413506	2.913043
C	0.386321	0.623298	3.630968
C	1.103318	0.297168	4.790942
H	1.622761	1.089754	5.349018
C	1.148074	-1.023472	5.261510
H	1.691705	-1.267150	6.186705
C	0.497893	-2.027199	4.541473
H	0.532181	-3.063133	4.914694
C	-0.223567	-1.764191	3.357967
C	0.359948	2.056730	3.109448
H	-0.619047	2.211997	2.614701
C	0.492606	3.121486	4.204720
H	-0.249155	2.969977	5.014940
H	0.332105	4.131711	3.776910
H	1.501466	3.122581	4.667099
C	1.428290	2.259450	2.025149
H	1.312127	1.522835	1.197287
H	2.452331	2.133304	2.433897
H	1.355745	3.268976	1.574913
C	-0.864247	-2.995581	2.701005
H	-1.376982	-3.528260	3.535186
C	-1.930086	-2.784817	1.616947
H	-2.787168	-2.185717	1.974785
H	-2.315758	-3.771057	1.286290
H	-1.530819	-2.254199	0.729973
C	0.244773	-3.938160	2.191097
H	0.959785	-4.207933	2.992300
H	0.834286	-3.449029	1.394737
H	-0.185650	-4.874338	1.779933
P	1.823115	-1.266035	-0.671034
C	1.537628	-2.813806	-1.659140
C	0.421657	-3.603050	-1.318098
H	-0.279736	-3.241241	-0.554215
C	0.196970	-4.837625	-1.941507
H	-0.677090	-5.442023	-1.654352
C	1.072416	-5.289264	-2.941403
H	0.891962	-6.252508	-3.442291
C	2.175214	-4.500420	-3.305100
H	2.864460	-4.844668	-4.091488
C	2.413714	-3.274042	-2.663537
H	3.291564	-2.674193	-2.944332
C	2.847795	-1.951783	0.722705
C	3.557311	-3.165919	0.619972
H	3.496891	-3.762201	-0.301888
C	4.334286	-3.623091	1.694611
H	4.876789	-4.576980	1.605977
C	4.422259	-2.870156	2.877059
H	5.032297	-3.232670	3.718579
C	3.723950	-1.657812	2.983173
H	3.772117	-1.063026	3.906728
C	2.934603	-1.207183	1.915147
H	2.365031	-0.273346	2.011970
C	3.144616	-0.424475	-1.659683
C	4.378080	-0.048690	-1.087780
H	4.601521	-0.308041	-0.042725
C	5.325725	0.655389	-1.846387
H	6.283337	0.943790	-1.386216
C	5.060797	0.981178	-3.185918
H	5.807804	1.528719	-3.780713
C	3.835400	0.606782	-3.760114
H	3.606618	0.864164	-4.805379
C	2.878609	-0.080459	-3.001181
H	1.916380	-0.351003	-3.459711

Conformation 30.
Multiplicity: 3
Charge: 0
E(B97-3c) = -3893.563746418426 Hartree
E(M06/def2-TZVP) = -3893.294304769163 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3891.978335656992 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3892.238782841677 Hartree
E(PBEh-3c) = -3888.297791553374 Hartree
E(PM6) = 84.72964 Kcal/mol
E(PM7) = 39.87404 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3895.855128730957 Hartree
E(GFN1-xTB) = -161.270180153085 Hartree
E(GFN2-xTB) = -160.182244923714 Hartree
E(GFN-FF) = -22.399762225851 Hartree

Coordinates:

Co	-0.313747	0.051608	-0.068013
N	1.147533	-0.859228	0.924850
N	-1.020207	1.135697	1.355752
C	2.307882	-1.407810	3.204964
C	1.369049	-0.586641	2.229665
C	0.654220	0.428840	2.916019
H	1.001424	0.587335	3.934772
C	-0.452074	1.234629	2.573956
C	-0.859322	2.268446	3.682579
C	3.080707	-0.475993	4.178336
H	3.774357	-1.088060	4.789201
H	2.428364	0.061483	4.892016
H	3.687170	0.276207	3.636873
C	1.354560	-2.296222	4.045826
H	1.937130	-2.933094	4.744386
H	0.754143	-2.963216	3.398547
H	0.648369	-1.681802	4.637947
C	3.382562	-2.321856	2.578855
H	3.972129	-2.770493	3.404558
H	4.084352	-1.772260	1.927116
H	2.963875	-3.150678	1.987210
C	0.178076	3.416106	3.597217
H	-0.055226	4.207642	4.340424
H	0.176268	3.879850	2.592292
H	1.203316	3.045132	3.793884
C	-2.273684	2.871193	3.564287
H	-2.439796	3.545349	4.429508
H	-3.062585	2.097379	3.583688
H	-2.420826	3.466360	2.649269
C	-0.785577	1.644597	5.100064
H	-1.161101	2.379738	5.840354
H	0.242284	1.378079	5.411774
H	-1.412853	0.735344	5.175978
C	1.953926	-1.750931	0.164839
C	1.614512	-3.130232	0.039714
C	2.491733	-3.989713	-0.645279
H	2.237109	-5.057770	-0.724644
C	3.681519	-3.519381	-1.209905
H	4.371474	-4.212409	-1.715403
C	3.969089	-2.148427	-1.153719
H	4.881459	-1.772266	-1.637412
C	3.117467	-1.242349	-0.495358
C	0.340443	-3.708447	0.641401
H	-0.081409	-2.934789	1.313489
C	-0.692614	-3.989779	-0.462049
H	-0.946841	-3.067644	-1.015111
H	-1.626347	-4.411693	-0.037076
H	-0.297026	-4.715771	-1.201919
C	0.584995	-4.973766	1.480213
H	-0.346728	-5.272570	2.003635
H	1.371874	-4.822577	2.245316
H	0.892123	-5.831850	0.847450
C	3.417409	0.253651	-0.513646

H	2.420365	0.739892	-0.600401
C	4.059045	0.785009	0.778945
H	3.397921	0.648403	1.652384
H	4.261710	1.872133	0.684549
H	5.026163	0.279214	0.982769
C	4.272872	0.675909	-1.713661
H	4.330887	1.779945	-1.770583
H	3.857805	0.312294	-2.673469
H	5.313615	0.300423	-1.621859
C	-2.314182	1.586366	0.980224
C	-2.496872	2.822506	0.285695
C	-3.800618	3.242949	-0.031320
H	-3.937656	4.202714	-0.552968
C	-4.920643	2.474905	0.301429
H	-5.934438	2.830004	0.061926
C	-4.730464	1.230188	0.915066
H	-5.601551	0.595497	1.145715
C	-3.449747	0.752479	1.247806
C	-1.326578	3.709857	-0.122712
H	-0.398762	3.184410	0.191715
C	-1.299181	3.898794	-1.649442
H	-1.316098	2.930031	-2.180967
H	-0.394630	4.456215	-1.966796
H	-2.181778	4.477931	-1.991359
C	-1.354631	5.086055	0.566973
H	-1.380533	5.006579	1.669959
H	-2.245165	5.669654	0.254062
H	-0.457379	5.677542	0.290699
C	-3.365640	-0.669221	1.806302
H	-4.415655	-1.034559	1.785472
C	-2.571417	-1.609988	0.891140
H	-2.938824	-1.594480	-0.152538
H	-2.639269	-2.656701	1.248423
H	-1.479844	-1.363247	0.905704
C	-2.892017	-0.812301	3.262260
H	-3.429162	-0.119796	3.940358
H	-1.804606	-0.627189	3.359437
H	-3.086162	-1.845891	3.616975
P	-0.237454	-0.152440	-2.285693
C	1.031797	0.868325	-3.175744
C	1.394761	2.096317	-2.588571
H	1.005073	2.348802	-1.590920
C	2.241912	2.987818	-3.260349
H	2.505801	3.948220	-2.792042
C	2.763565	2.648759	-4.519011
H	3.435866	3.343403	-5.044728
C	2.433552	1.413728	-5.098856
H	2.849019	1.135021	-6.079708
C	1.566027	0.529987	-4.436331
H	1.298716	-0.428762	-4.904574
C	-1.792226	0.541870	-3.047074
C	-1.823680	1.076315	-4.352289
H	-0.901580	1.125361	-4.949884
C	-3.026459	1.554936	-4.891718
H	-3.036244	1.975250	-5.909324
C	-4.212821	1.499278	-4.140823
H	-5.154235	1.877391	-4.567218
C	-4.189738	0.967958	-2.843436
H	-5.104096	0.930088	-2.234097
C	-2.984261	0.500185	-2.299833
H	-2.964435	0.117154	-1.271020
C	-0.144594	-1.770292	-3.183775
C	-1.293264	-2.372575	-3.738846
H	-2.257728	-1.844511	-3.711130
C	-1.212755	-3.641698	-4.331721
H	-2.117878	-4.097999	-4.761226
C	0.014618	-4.320911	-4.387902
H	0.077123	-5.313781	-4.858409
C	1.160730	-3.726163	-3.836468
H	2.129297	-4.248078	-3.860439
C	1.081489	-2.466152	-3.228567
H	1.983972	-2.024504	-2.782065

Conformation 31.
Multiplicity: 3
Charge: 0
E(B97-3c) = -3893.567685664138 Hartree
E(M06/def2-TZVP) = -3893.299025540857 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3891.981626915445 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3892.243500924945 Hartree
E(PBEh-3c) = -3888.300583467721 Hartree
E(PM6) = 82.74895 Kcal/mol
E(PM7) = 38.42901 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3895.860393132127 Hartree
E(GFN1-xTB) = -161.277079756721 Hartree
E(GFN2-xTB) = -160.190653523218 Hartree
E(GFN-FF) = -22.404095107430 Hartree

Coordinates:

Co	0.173462	-0.209516	0.122077
N	-0.571785	0.912887	-1.354090
N	-0.839855	-1.804060	-0.282236
C	-1.869082	1.176890	-3.605762
C	-1.377925	0.418189	-2.309043
C	-1.839604	-0.920775	-2.269864
H	-2.480720	-1.190465	-3.110811
C	-1.668221	-1.960302	-1.331094
C	-2.525565	-3.237008	-1.651318
C	-1.225184	0.462258	-4.821687
H	-1.562778	0.940334	-5.764798
H	-1.485424	-0.612354	-4.868668
H	-0.119948	0.536682	-4.781250
C	-3.412480	1.082595	-3.716610
H	-3.753228	1.636924	-4.615119
H	-3.903318	1.539954	-2.833742
H	-3.783490	0.044588	-3.808700
C	-1.532000	2.674763	-3.748868
H	-1.895427	3.008381	-4.742930
H	-0.451628	2.888256	-3.703825
H	-2.027411	3.301800	-2.987370
C	-2.094127	-3.785097	-3.033869
H	-2.702048	-4.676417	-3.294363
H	-1.029638	-4.095841	-3.015944
H	-2.214856	-3.044506	-3.847141
C	-2.445451	-4.423791	-0.670747
H	-3.136060	-5.210943	-1.037462
H	-2.757540	-4.158628	0.354585
H	-1.437812	-4.870287	-0.608496
C	-4.015854	-2.813174	-1.692700
H	-4.654430	-3.695124	-1.907249
H	-4.222984	-2.046283	-2.462736
H	-4.328041	-2.396057	-0.713622
C	-0.223366	2.279065	-1.243377
C	1.056155	2.755210	-1.650557
C	1.336805	4.126857	-1.467924
H	2.332758	4.499505	-1.756465
C	0.388400	5.021877	-0.961764
H	0.634111	6.089098	-0.854514
C	-0.875520	4.542961	-0.582672
H	-1.621361	5.243842	-0.181222
C	-1.191696	3.180891	-0.686808
C	2.152638	1.944732	-2.358698
H	3.091974	2.242000	-1.844194
C	2.094211	0.414720	-2.296793
H	1.956435	0.062870	-1.253240
H	3.055569	-0.005982	-2.656353
H	1.277984	-0.012048	-2.909280
C	2.310694	2.389850	-3.828596
H	3.214247	1.925993	-4.275462
H	2.411037	3.489203	-3.920477
H	1.440265	2.081466	-4.442346
C	-2.543798	2.642419	-0.230122
H	-2.847338	1.867423	-0.963478
C	-2.414048	1.926674	1.123813
H	-1.581078	1.193891	1.089795
H	-3.343835	1.377728	1.376695
H	-2.186055	2.639082	1.941290
C	-3.659894	3.690527	-0.192800
H	-4.631079	3.204577	0.031223
H	-3.759605	4.222110	-1.161279
H	-3.490543	4.451607	0.597274
C	-0.576269	-2.779574	0.713389
C	0.462929	-3.738189	0.509018
C	0.711732	-4.689228	1.511897
H	1.503704	-5.438119	1.361909
C	-0.035609	-4.707724	2.699138
H	0.164807	-5.470756	3.466661
C	-1.027511	-3.740942	2.907361
H	-1.598096	-3.742776	3.849174
C	-1.313279	-2.767716	1.933537
C	1.316130	-3.681703	-0.750348
H	0.709901	-3.179834	-1.532025
C	2.537055	-2.783317	-0.488601
H	2.195818	-1.787133	-0.132938
H	3.138970	-2.632697	-1.408279
H	3.189326	-3.212216	0.299908
C	1.730170	-5.056783	-1.287788
H	0.850858	-5.714326	-1.443821
H	2.426738	-5.580443	-0.600861
H	2.253805	-4.948747	-2.259258
C	-2.361288	-1.697427	2.205504
H	-2.482533	-1.120768	1.265711
C	-3.732534	-2.277935	2.581341
H	-4.112154	-2.968364	1.801422
H	-4.475654	-1.463649	2.705691
H	-3.695478	-2.838940	3.538320
C	-1.846046	-0.723322	3.278269
H	-0.900929	-0.249576	2.948010
H	-1.643136	-1.244803	4.236612
H	-2.575798	0.087960	3.472868
P	1.613228	0.811292	1.526097
C	2.401526	-0.315754	2.778152

C	3.480070	0.150805	3.562878
H	3.859621	1.173342	3.415403
C	4.066202	-0.679969	4.525749
H	4.905982	-0.305612	5.131205
C	3.585548	-1.988063	4.716128
H	4.049968	-2.641499	5.470692
C	2.515930	-2.456061	3.940928
H	2.127559	-3.476185	4.074356
C	1.926378	-1.622244	2.974939
H	1.090087	-1.994987	2.369898
C	0.916593	2.106667	2.649224
C	0.610289	1.817498	3.996839
H	0.874497	0.838910	4.422081
C	-0.030681	2.772090	4.800651
H	-0.265445	2.528196	5.848188
C	-0.364657	4.032092	4.278520
H	-0.862502	4.780648	4.913589
C	-0.063658	4.325592	2.939479
H	-0.328375	5.302564	2.506669
C	0.558586	3.366316	2.128101
H	0.747838	3.600636	1.074193
C	3.185306	1.559846	0.864054
C	3.510136	2.928933	0.887351
H	2.834784	3.652030	1.362270
C	4.706759	3.386380	0.310076
H	4.941118	4.461744	0.335184
C	5.598109	2.485130	-0.290425
H	6.532262	2.847840	-0.745375
C	5.294734	1.112867	-0.293048
H	5.993171	0.391236	-0.743663
C	4.101263	0.656161	0.279501
H	3.878536	-0.421412	0.282080

Conformation 33.
Multiplicity: 3
Charge: 0
E(B97-3c) = -3893.560975757845 Hartree
E(M06/def2-TZVP) = -3893.293048516383 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3891.975968812902 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3892.237063850715 Hartree
E(PBEh-3c) = -3888.290290971566 Hartree
E(PM6) = 89.87465 Kcal/mol
E(PM7) = 44.26548 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3895.851085675509 Hartree
E(GFN1-xTB) = -161.271474674767 Hartree
E(GFN2-xTB) = -160.182984676831 Hartree
E(GFN-FF) = -22.392301594608 Hartree

Coordinates:

Co	0.087454	-0.233351	0.313362
N	-0.866734	0.756632	-1.156659
N	-0.682750	-1.977049	-0.057434
C	-2.252776	0.761238	-3.377266
C	-1.578541	0.116829	-2.100766
C	-1.801576	-1.283351	-2.051539
H	-2.385390	-1.662690	-2.890785
C	-1.451663	-2.280815	-1.117617
C	-2.030905	-3.701684	-1.469226
C	-1.655203	0.090000	-4.641324
H	-2.117396	0.528706	-5.549799
H	-1.825548	-1.002694	-4.671866
H	-0.561958	0.259155	-4.704067
C	-3.774825	0.469196	-3.325280
H	-4.280033	0.952908	-4.186971
H	-4.225864	0.870142	-2.396880
H	-4.007471	-0.611678	-3.364914
C	-2.107473	2.281139	-3.595823
H	-2.627035	2.536178	-4.542573
H	-1.059176	2.606565	-3.694726
H	-2.564162	2.883525	-2.793834
C	-1.336346	-4.197484	-2.761276
H	-1.742504	-5.188217	-3.053901
H	-0.244329	-4.312021	-2.611992
H	-1.488618	-3.501300	-3.608730
C	-1.869841	-4.804238	-0.403774
H	-2.405048	-5.707732	-0.761461
H	-2.304577	-4.522543	0.572367
H	-0.819436	-5.092025	-0.228946
C	-3.554616	-3.591575	-1.737811
H	-3.961663	-4.597434	-1.968840
H	-3.799483	-2.932969	-2.591969
H	-4.089561	-3.203567	-0.849824
C	-0.640931	2.156848	-1.150985
C	0.529249	2.717801	-1.750672
C	0.697709	4.117579	-1.685901
H	1.609619	4.554595	-2.123351
C	-0.256401	4.963062	-1.108778
H	-0.101310	6.052443	-1.099726
C	-1.399665	4.400374	-0.527003
H	-2.149335	5.055949	-0.056788
C	-1.597885	3.010453	-0.508805
C	1.630752	1.969387	-2.523902
H	2.575720	2.358015	-2.086855
C	1.710566	0.443484	-2.412222
H	1.657860	0.119786	-1.353582
H	2.682522	0.098283	-2.819682
H	0.902920	-0.078825	-2.958915
C	1.656709	2.373473	-4.014002
H	2.570206	1.973344	-4.500002
H	1.652778	3.472634	-4.149623
H	0.783611	1.964314	-4.560255
C	-2.841208	2.453476	0.182651
H	-2.817427	1.351362	0.060933
C	-2.831776	2.769125	1.688575
H	-1.902727	2.426561	2.178477
H	-3.695638	2.287982	2.192854
H	-2.910179	3.861455	1.867128
C	-4.150750	2.974385	-0.436615
H	-5.026155	2.499818	0.052838
H	-4.217561	2.768120	-1.521541
H	-4.249986	4.071263	-0.299278
C	-0.309223	-2.844542	0.995720
C	0.825913	-3.702208	0.851115
C	1.186950	-4.541167	1.917331
H	2.054899	-5.207776	1.807752
C	0.460652	-4.546484	3.116330
H	0.746896	-5.221563	3.936962
C	-0.621249	-3.669507	3.267395
H	-1.177079	-3.644680	4.218490
C	-1.020735	-2.802701	2.233017
C	1.650370	-3.661144	-0.428029
H	0.965956	-3.350181	-1.242451
C	2.716882	-2.561804	-0.308823
H	2.219494	-1.595279	-0.077135
H	3.283014	-2.439190	-1.255273
H	3.431453	-2.780097	0.511252
C	2.265328	-5.008019	-0.824459
H	1.500354	-5.809681	-0.872863
H	3.052084	-5.334335	-0.113076
H	2.743816	-4.931922	-1.821922
C	-2.144894	-1.811715	2.521527
H	-2.466645	-2.043840	3.560178
C	-1.641589	-0.362181	2.548253
H	-0.724588	-0.243421	3.155070
H	-2.410234	0.311176	2.975460
H	-1.471168	0.038273	1.510883
C	-3.394768	-1.929101	1.634314
H	-3.769759	-2.970873	1.590728
H	-3.193059	-1.584814	0.601823
H	-4.207973	-1.295935	2.045688
P	1.625722	0.982187	1.434962
C	3.069040	1.768798	0.558088
C	3.959690	0.883187	-0.088864
H	3.792851	-0.200668	-0.020574
C	5.058638	1.366895	-0.809539
H	5.736472	0.657104	-1.307921
C	5.293372	2.749438	-0.895238
H	6.152052	3.132629	-1.467126
C	4.431592	3.635476	-0.232323
H	4.614597	4.720221	-0.274039
C	3.330602	3.150692	0.493490
H	2.679413	3.864149	1.014134
C	2.599835	-0.005683	2.676797
C	2.172881	-1.286541	3.065949
H	1.276157	-1.728068	2.610367
C	2.888800	-2.011930	4.034209
H	2.537023	-3.014253	4.318850
C	4.038726	-1.462512	4.617447
H	4.602653	-2.032101	5.372128
C	4.471864	-0.180993	4.233223
H	5.374035	0.256842	4.687586
C	3.758064	0.543259	3.270049
H	4.100648	1.546314	2.973652
C	0.985239	2.322059	2.542742
C	0.539761	3.540788	1.990380
H	0.602386	3.712260	0.909146
C	-0.006418	4.539924	2.808129
H	-0.337984	5.484322	2.349956
C	-0.155887	4.324328	4.186409
H	-0.595695	5.103791	4.827003
C	0.250844	3.099976	4.740741
H	0.131207	2.914886	5.819383
C	0.824711	2.109036	3.929839
H	1.159776	1.164554	4.382878

Conformation 7.
Multiplicity: 3
Charge: 0
E(B97-3c) = -3893.568404119551 Hartree
E(M06/def2-TZVP) = -3893.297187092774 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3891.983218186719 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3892.244056380075 Hartree

E(PBEh-3c) = -3888.303860858014 Hartree
E(PM6) = 81.92260 Kcal/mol
E(PM7) = 42.27180 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3895.861159013871 Hartree
E(GFN1-xTB) = -161.277616075449 Hartree
E(GFN2-xTB) = -160.191278104577 Hartree
E(GFN-FF) = -22.407544264399 Hartree

Coordinates:

Co	-0.138952	-0.048740	-0.094793
N	1.787715	-0.451862	0.080884
N	0.015544	1.476534	-1.245135
C	4.275924	-0.094617	-0.649100
C	2.725024	0.225306	-0.619242
C	2.388677	1.306222	-1.468679
H	3.248381	1.754246	-1.969055
C	1.164292	1.948127	-1.762229
C	1.316631	3.222924	-2.667072
C	4.658395	-0.417133	-2.119772
H	5.742373	-0.646357	-2.180722
H	4.449986	0.419481	-2.812456
H	4.105605	-1.302635	-2.490346
C	5.080793	1.148073	-0.194394
H	6.167099	0.935247	-0.270884
H	4.865596	1.406457	0.861115
H	4.870454	2.043379	-0.810638
C	4.786421	-1.282887	0.191985
H	5.863669	-1.419006	-0.036971
H	4.276157	-2.230511	-0.047919
H	4.695958	-1.117934	1.278989
C	2.178316	2.897847	-3.915003
H	2.262689	3.805957	-4.546133
H	1.713268	2.102564	-4.529642
H	3.207015	2.576442	-3.666117
C	0.013163	3.845477	-3.205524
H	0.283591	4.682157	-3.881812
H	-0.632896	4.255784	-2.412079
H	-0.592001	3.126575	-3.786990
C	2.051954	4.297355	-1.828478
H	2.174173	5.227449	-2.422326
H	3.056925	3.954378	-1.514118
H	1.483383	4.550672	-0.913055
C	2.110478	-1.268658	1.192667
C	1.962612	-2.686445	1.130265
C	2.386643	-3.455135	2.227194
H	2.298544	-4.549727	2.182895
C	2.913959	-2.857924	3.378896
H	3.252443	-3.481821	4.219749
C	2.968654	-1.460370	3.469627
H	3.346382	-0.994341	4.391268
C	2.565240	-0.646061	2.397459
C	1.328883	-3.330913	-0.093825
H	0.504389	-2.625732	-0.352391
C	2.244933	-3.388750	-1.327111
H	2.589204	-2.382051	-1.624443
H	1.699275	-3.825856	-2.189786
H	3.135297	-4.024154	-1.138105
C	0.723392	-4.710405	0.181968
H	0.133165	-5.052859	-0.692144
H	0.051773	-4.697542	1.061668
H	1.510390	-5.473506	0.357955
C	2.571956	0.875266	2.511979
H	2.885866	1.283686	1.530380
C	1.147065	1.395716	2.748765
H	0.453945	1.001026	1.972767
H	1.107811	2.502018	2.702701
H	0.754976	1.077128	3.737108
C	3.539802	1.426877	3.563208
H	3.568871	2.534249	3.514100
H	4.571164	1.050073	3.407621
H	3.233726	1.156049	4.595175
C	-1.296961	1.973433	-1.454534
C	-1.806488	3.046219	-0.662456
C	-3.087222	3.549921	-0.947673
H	-3.476316	4.389504	-0.351473
C	-3.873409	3.006574	-1.969428
H	-4.864554	3.428937	-2.194363
C	-3.406927	1.888885	-2.676596
H	-4.053229	1.428098	-3.436616
C	-2.138207	1.338002	-2.425648
C	-1.014790	3.632314	0.500453
H	0.008684	3.206556	0.450122
C	-0.900954	5.164477	0.439317
H	-0.496002	5.513578	-0.530911
H	-0.231713	5.536048	1.242255
H	-1.886917	5.652403	0.584167
C	-1.638431	3.190979	1.836499
H	-1.669630	2.088458	1.921906
H	-2.681658	3.555706	1.930366
H	-1.059514	3.589148	2.694765
C	-1.686618	0.058390	-3.124710
H	-1.181613	-0.533904	-2.320935
C	-2.850919	-0.783253	-3.656606
H	-3.606203	-0.995906	-2.874235
H	-2.476222	-1.755543	-4.030745
H	-3.360689	-0.283213	-4.506588
C	-0.650142	0.289787	-4.235351
H	0.260832	0.779210	-3.849222
H	-1.072645	0.922544	-5.043804
H	-0.346001	-0.677023	-4.686865
P	-1.694636	-1.321365	0.853363
C	-2.687894	-2.417500	-0.276256
C	-4.069008	-2.635472	-0.081967
H	-4.591891	-2.122448	0.738502
C	-4.779200	-3.503852	-0.925051
H	-5.856839	-3.659259	-0.762395
C	-4.119595	-4.177468	-1.965732
H	-4.677334	-4.861357	-2.623432
C	-2.746821	-3.967638	-2.166057
H	-2.220740	-4.483892	-2.983599
C	-2.041224	-3.084962	-1.335207
H	-0.970746	-2.910176	-1.514271
C	-3.030972	-0.236376	1.555577
C	-3.252137	-0.107298	2.942086
H	-2.657215	-0.699493	3.652017
C	-4.237328	0.768275	3.425755
H	-4.394891	0.858990	4.511537
C	-5.025334	1.511788	2.534184
H	-5.802261	2.191844	2.915503
C	-4.812894	1.383732	1.152069
H	-5.414627	1.965350	0.438228
C	-3.816811	0.527169	0.665190
H	-3.650808	0.459867	-0.420374
C	-1.389161	-2.457228	2.283834
C	-2.012326	-3.713770	2.425084
H	-2.697576	-4.080068	1.647208
C	-1.758085	-4.505100	3.556123
H	-2.245711	-5.487506	3.651901
C	-0.891027	-4.047481	4.561012
H	-0.694443	-4.670546	5.446881
C	-0.267446	-2.797705	4.424303
H	0.432107	-2.436205	5.192115
C	-0.504774	-2.014005	3.286800
H	0.018146	-1.055934	3.164019

WUDYOL

Conformation 0.
Multiplicity: 2
Charge: 0
E(B97-3c) = -3367.159382788117 Hartree
E(M06/def2-TZVP) = -3366.992280859620 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3365.968433722718 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3366.034036672497 Hartree
E(PBEh-3c) = -3362.577014132278 Hartree
E(PM6) = 65.51977 Kcal/mol
E(PM7) = 111.42633 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3368.997914549946 Hartree
E(GFN1-xTB) = -130.537921840998 Hartree
E(GFN2-xTB) = -127.373494875306 Hartree
E(GFN-FF) = -15.779968118754 Hartree

Coordinates:

Co	0.341013	0.113855	-0.487642
N	-0.075237	-1.560856	-1.426005
O	-4.499134	-2.980696	1.497517
O	-4.262037	-1.995241	3.533288
C	-1.841110	0.832557	1.483856
C	1.651714	-1.541399	-3.199741
N	0.734389	1.818529	0.398168
C	-1.947420	-2.377129	-0.031781
H	-2.681466	-3.177118	0.129091
C	-2.055820	-1.239553	0.764479
C	3.703608	-0.111425	-3.065595
H	4.250731	-0.599106	-3.878587
C	2.186980	-2.186930	-4.433841
N	1.973833	0.303956	-1.559455
C	2.653988	-3.519287	-4.418875
H	2.623779	-4.085865	-3.476158
C	2.764940	-2.052203	-6.806212
H	2.803205	-1.473087	-7.741458
C	2.253641	-1.460059	-5.642264
H	1.891459	-0.421098	-5.660861
C	3.166838	-4.110141	-5.582848
H	3.532881	-5.147746	-5.552004
C	4.223585	3.141545	-0.337265
C	3.221974	-3.379379	-6.780415
H	3.624036	-3.843831	-7.693581
C	4.650452	3.926134	-1.430494
H	4.083884	3.884868	-2.372880
C	6.483224	4.826856	-0.108142

H	7.362924	5.482203	-0.019288
C	4.943269	3.220603	0.874669
H	4.615301	2.612289	1.731061
C	6.065112	4.054752	0.987280
H	6.618569	4.099227	1.937656
C	5.771338	4.761429	-1.316463
H	6.086966	5.371197	-2.176779
C	-3.105522	-1.036081	1.739198
C	-1.071571	-2.472445	-1.103797
C	3.030937	1.179525	-1.336226
C	0.496979	-2.052838	-2.589715
C	-1.139844	-3.529522	-2.085129
H	-1.856481	-4.358306	-2.051026
C	2.372548	-0.477456	-2.634775
C	-0.121255	2.549725	1.212490
C	4.124697	0.895360	-2.238691
H	5.088510	1.413633	-2.235397
C	0.486804	3.798779	1.607350
H	0.000063	4.550140	2.239942
C	1.887620	2.580734	0.315671
C	-0.190768	-3.249967	-3.031525
H	0.045182	-3.804524	-3.945114
C	-3.000553	0.285090	2.156746
C	1.745072	3.811415	1.067531
H	2.515787	4.585077	1.144008
C	-1.345191	2.115999	1.700734
H	-1.903634	2.765090	2.386948
C	3.024679	2.259446	-0.441487
N	-1.272067	-0.105557	0.640876
C	-4.035362	-2.094656	2.200627
C	-3.904282	1.063319	3.034904
O	-3.567182	2.011896	3.730208
O	-5.187722	0.633076	2.925563
C	-6.159390	1.314822	3.746010
H	-7.112635	1.217988	3.190410
H	-5.879889	2.385791	3.810960
C	-5.176717	-2.951087	4.104967
H	-5.058026	-3.920906	3.580085
H	-6.213166	-2.598950	3.905589
C	-6.254541	0.698726	5.132620
H	-6.534060	-0.371557	5.078165
H	-7.025427	1.227222	5.729101
H	-5.287378	0.787410	5.664597
C	-4.888903	-3.051242	5.589343
H	-3.856717	-3.412567	5.767003
H	-5.592806	-3.762648	6.065237
H	-4.999192	-2.067808	6.087567

Conformation 16.
Multiplicity: 2
Charge: 0
E(B97-3c) = converged!) Hartree
E(M06/def2-TZVP) = -3366.992755779787 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3365.969028660086 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3366.035072868632 Hartree
E(PBEh-3c) = -3362.578405776997 Hartree
E(PM6) = 66.49799 Kcal/mol
E(PM7) = 111.32898 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3368.999458609018 Hartree
E(GFN1-xTB) = -130.536871835805 Hartree
E(GFN2-xTB) = -127.373131539602 Hartree
E(GFN-FF) = -15.779520085293 Hartree

Coordinates:

Co	-0.118933	0.558760	0.187646
N	0.929731	0.314755	1.831395
O	2.544749	-4.846189	0.947708
O	1.109161	-5.780035	-0.538752
C	0.233181	-1.786510	-1.690206
C	0.780993	2.580355	2.817137
N	-1.137944	0.830647	-1.466642
C	1.519281	-2.076623	1.608507
H	2.031912	-2.934244	2.062618
C	1.021321	-2.239018	0.317827
C	-0.949883	4.246616	2.114400
H	-0.786036	4.951506	2.935627
C	1.232789	3.509237	3.894048
N	-0.674315	2.333564	0.811366
C	1.945019	4.682805	3.565295
H	2.171143	4.891689	2.508761
C	1.366761	4.135925	6.253545
H	1.129111	3.921320	7.306651
C	0.945565	3.249508	5.251585
H	0.373151	2.347358	5.514760
C	2.367366	5.567814	4.567966
H	2.927851	6.474771	4.294453
C	-3.415557	3.875670	-1.360580
C	2.080889	5.296397	5.915211
H	2.411994	5.991111	6.701961
C	-3.088711	5.212440	-1.675789
H	-2.042003	5.540942	-1.590929
C	-5.410338	5.681984	-2.230206
H	-6.186789	6.385076	-2.567866
C	-4.756923	3.457096	-1.494447
H	-5.019409	2.416583	-1.250524
C	-5.746261	4.353746	-1.923966
H	-6.788580	4.012388	-2.016494
C	-4.078327	6.107966	-2.106571
H	-3.805256	7.145206	-2.353817
C	1.198298	-3.440328	-0.469669
C	1.537177	-0.855322	2.266759
C	-1.688815	3.130830	0.292431
C	1.283380	1.271953	2.770148
C	2.288167	-0.625883	3.478783
H	2.861570	-1.397335	4.005792
C	-0.205357	3.022076	1.921389
C	-1.078776	0.056150	-2.618450
C	-1.892953	4.297018	1.123157
H	-2.661852	5.057490	0.955793
C	-1.917352	0.610717	-3.655193
H	-2.026386	0.181090	-4.657766
C	-2.033038	1.844730	-1.763527
C	2.164654	0.705731	3.772081
H	2.611448	1.267341	4.598326
C	0.746133	-3.137837	-1.749171
C	-2.528550	1.712328	-3.118984
H	-3.238520	2.399410	-3.590371
C	-0.407525	-1.150392	-2.750980
H	-0.479074	-1.695714	-3.700524
C	-2.367332	2.911565	-0.915220
N	0.409199	-1.246849	-0.428003
C	1.713350	-4.725365	0.058738
C	0.804543	-3.960613	-2.980743
O	-0.007831	-3.926996	-3.894336
O	1.912052	-4.739917	-3.001689
C	2.019351	-5.645575	-4.116426
H	1.983597	-5.063081	-5.061311
H	1.129403	-6.311740	-4.121305
C	1.596703	-7.080923	-0.159283
H	1.460452	-7.213088	0.935134
H	2.691013	-7.122633	-0.349229
C	3.313870	-6.417510	-3.964223
H	4.184403	-5.732417	-3.949202
H	3.439561	-7.120727	-4.811122
H	3.321997	-7.003255	-3.023241
C	0.833490	-8.113988	-0.962649
H	-0.254894	-8.043020	-0.768365
H	1.169813	-9.133638	-0.689271
H	0.997929	-7.974901	-2.049957

Conformation 19.
Multiplicity: 2
Charge: 0
E(B97-3c) = -3367.158645434764 Hartree
E(M06/def2-TZVP) = -3366.992065531022 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3365.967817113296 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3366.033339476244 Hartree
E(PBEh-3c) = -3362.576796724290 Hartree
E(PM6) = 64.33428 Kcal/mol
E(PM7) = 110.92964 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3368.996388442925 Hartree
E(GFN1-xTB) = -130.539912437967 Hartree
E(GFN2-xTB) = -127.374030582060 Hartree
E(GFN-FF) = -15.783350483146 Hartree

Coordinates:

Co	-0.155954	0.564459	0.005685
N	0.879508	0.764894	1.654840
O	3.336556	-4.045908	1.690732
O	3.236691	-5.017685	-0.357162
C	0.069683	-2.246691	-1.087189
C	-0.066657	2.876640	2.542636
N	-1.157831	0.397655	-1.672848
C	2.252474	-1.287605	1.549980
H	3.045510	-1.876659	2.026768
C	1.543959	-1.888577	0.510781
C	-1.605773	4.358232	1.224029
H	-1.769836	5.113404	1.998953
C	-0.099353	3.817167	3.700480
N	-0.868709	2.374609	0.244321
C	0.385605	5.137890	3.584475
H	0.794490	5.475291	2.620220
C	-0.621596	4.256238	6.048768
H	-1.020711	3.906068	7.012932
C	-0.599460	3.386783	4.948536
H	-0.978901	2.358396	5.045994
C	0.364716	6.006181	4.685755
H	0.752646	7.030828	4.579877
C	-2.674273	3.700308	-2.838737
C	-0.140315	5.568785	5.920581
H	-0.156436	6.250721	6.784266
C	-1.996073	4.853413	-3.289864

H	-0.945532	5.003011	-2.998373
C	-3.984230	5.597119	-4.477610
H	-4.494041	6.334602	-5.115920
C	-4.022247	3.516801	-3.216288
H	-4.564688	2.631675	-2.851522
C	-4.671100	4.457628	-4.029302
H	-5.724357	4.302520	-4.308890
C	-2.645088	5.792680	-4.104376
H	-2.099187	6.682763	-4.452661
C	1.738395	-3.257745	0.078128
C	1.902698	-0.063096	2.099165
C	-1.608297	3.116463	-0.665572
C	0.795539	1.770691	2.602335
C	2.489694	0.452388	3.314190
H	3.321959	-0.021131	3.847884
C	-0.828973	3.150814	1.397945
C	-1.340118	-0.757068	-2.421336
C	-2.060367	4.353168	-0.067469
H	-2.682290	5.097957	-0.574082
C	-2.058657	-0.471576	-3.641388
H	-2.312557	-1.222015	-4.399082
C	-1.773390	1.400888	-2.406023
C	1.787126	1.580866	3.642234
H	1.926408	2.251235	4.496387
C	0.774275	-3.498346	-0.897635
C	-2.293517	0.877215	-3.653731
H	-2.788698	1.476954	-4.423800
C	-0.845130	-2.015769	-2.112987
H	-1.075983	-2.855415	-2.780422
C	-1.974921	2.716444	-1.961666
N	0.525635	-1.284133	-0.204083
C	2.824180	-4.132646	0.581797
C	0.425839	-4.751491	-1.611120
O	-0.030838	-4.805774	-2.746012
O	0.611571	-5.844458	-0.833746
C	0.321264	-7.115880	-1.453920
H	-0.636747	-7.032102	-2.007082
H	0.188008	-7.809917	-0.601226
C	4.268032	-5.939953	0.055299
H	5.049475	-5.377547	0.606493
H	4.694162	-6.314498	-0.895853
C	1.435503	-7.574244	-2.382665
H	1.539893	-6.879073	-3.237124
H	1.199427	-8.581053	-2.782741
H	2.405021	-7.631615	-1.850726
C	3.720965	-7.072254	0.911358
H	3.323979	-6.679695	1.866578
H	4.530949	-7.792990	1.143629
H	2.910996	-7.617236	0.388202

Conformation 20.
Multiplicity: 2
Charge: 0
E(B97-3c) = -3367.157770368557 Hartree
E(M06/def2-TZVP) = -3366.989652078966 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3365.966264661020 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3366.031993362115 Hartree
E(PBEh-3c) = -3362.575336082713 Hartree
E(PM6) = 66.96457 Kcal/mol
E(PM7) = 112.31984 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3368.997505453103 Hartree
E(GFN1-xTB) = -130.535278876975 Hartree
E(GFN2-xTB) = -127.370837819746 Hartree
E(GFN-FF) = -15.777239715432 Hartree

Coordinates:

Co	0.176251	0.451465	0.164384
N	-0.355268	-0.463877	1.820653
O	2.671290	-5.568840	-0.608473
O	0.457046	-5.493827	-0.112872
C	1.742223	-1.394655	-1.658225
C	-1.244887	1.432565	3.141628
N	0.769822	1.399734	-1.448300
C	0.217402	-2.793868	1.223514
H	0.182066	-3.840468	1.547580
C	0.800580	-2.511683	-0.009808
C	-1.866845	3.626435	2.109352
H	-2.406283	4.023677	2.974984
C	-1.787950	1.899328	4.450757
N	-0.657517	2.106863	0.817524
C	-2.991544	1.376104	4.971315
H	-3.537486	0.613420	4.395770
C	-1.615814	3.349643	6.412472
H	-1.070240	4.122197	6.975578
C	-1.109449	2.895367	5.185985
H	-0.171079	3.308485	4.786074
C	-3.498369	1.832277	6.196991
H	-4.441613	1.418311	6.585027
C	-0.720107	4.880359	-1.811932
C	-2.811370	2.818834	6.922324
H	-3.209512	3.175877	7.884247
C	-1.459927	4.930310	-3.013446
H	-1.811679	3.989537	-3.463234
C	-1.304572	7.357779	-3.045686
H	-1.532099	8.321824	-3.525397
C	-0.273263	6.092130	-1.241805
H	0.319035	6.061040	-0.314943
C	-0.563298	7.320282	-1.853872
H	-0.201468	8.255151	-1.399207
C	-1.751403	6.158857	-3.623820
H	-2.334868	6.179707	-4.556933
C	1.475676	-3.494166	-0.831431
C	-0.254135	-1.821378	2.092674
C	-0.912458	3.266144	0.092619
C	-0.840980	0.098235	2.992133
C	-0.656689	-2.108006	3.449342
H	-0.652709	-3.107978	3.898838
C	-1.220673	2.333446	2.066161
C	1.663841	0.934073	-2.404282
C	-1.700921	4.192801	0.874147
H	-2.070122	5.157710	0.513069
C	1.949691	1.955185	-3.384809
H	2.639300	1.826782	-4.227219
C	0.456413	2.686912	-1.852726
C	-0.986578	-0.909581	4.023217
H	-1.316371	-0.709819	5.047485
C	2.080113	-2.787091	-1.863645
C	1.184119	3.041107	-3.054959
H	1.116664	4.010896	-3.558229
C	2.138509	-0.364445	-2.507681
H	2.824340	-0.623890	-3.324180
C	-0.403922	3.566695	-1.178979
N	0.949955	-1.238124	-0.535148
C	1.631084	-4.942827	-0.527358
C	2.862189	-3.306064	-3.009471
O	3.680602	-2.662168	-3.653423
O	2.539216	-4.592364	-3.278648
C	3.306031	-5.252324	-4.306368
H	3.348507	-6.311914	-3.985574
H	4.331179	-4.830874	-4.312750
C	0.517570	-6.894655	0.229770
H	1.276414	-7.038253	1.028502
H	0.880034	-7.460810	-0.654281
C	2.647436	-5.098452	-5.667658
H	1.609567	-5.486400	-5.654059
H	3.218238	-5.662911	-6.432510
H	2.624366	-4.033859	-5.970929
C	-0.867704	-7.328137	0.662940
H	-1.205530	-6.760536	1.553018
H	-0.864417	-8.405467	0.921984
H	-1.605655	-7.167832	-0.147790

Conformation 21.
Multiplicity: 2
Charge: 0
E(B97-3c) = -3367.157794361162 Hartree
E(M06/def2-TZVP) = -3366.990631836714 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3365.966807133785 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3366.032446827778 Hartree
E(PBEh-3c) = -3362.575285059553 Hartree
E(PM6) = 66.17919 Kcal/mol
E(PM7) = 111.82583 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3368.996799562360 Hartree
E(GFN1-xTB) = -130.536320680686 Hartree
E(GFN2-xTB) = -127.372058919929 Hartree
E(GFN-FF) = -15.778291512796 Hartree

Coordinates:

Co	-0.087975	-0.505802	-0.248083
N	1.590202	-1.403556	-0.721929
O	5.036760	2.641169	0.412672
O	4.018935	4.208668	1.700868
C	0.389861	2.402209	0.463700
C	0.728149	-3.473674	-1.779348
N	-1.773785	0.366226	0.255004
C	3.217156	0.281723	0.066193
H	4.277368	0.537481	0.187542
C	2.285796	1.289487	0.304178
C	-1.687035	-4.150807	-1.723312
H	-1.584682	-5.068311	-2.310830
C	1.086368	-4.710284	-2.533947
N	-1.080474	-2.130939	-0.727216
C	0.899345	-5.990362	-1.968825
H	0.483658	-6.071182	-0.953226
C	1.992920	-5.771527	-4.541656
H	2.419384	-5.680110	-5.552234
C	1.642117	-4.616157	-3.828145
H	1.791519	-3.621370	-4.274331
C	1.251865	-7.145174	-2.682327
H	1.105029	-8.135372	-2.224588
C	-4.730962	-2.042876	0.362569
C	1.797929	-7.039518	-3.971481

H	2.074315	-7.946016	-4.531044
C	-5.837810	-1.500347	-0.325733
H	-5.670927	-0.695702	-1.057484
C	-7.340861	-3.030751	0.822424
H	-8.356605	-3.414668	1.001600
C	-4.952522	-3.093046	1.279495
H	-4.093739	-3.521193	1.818189
C	-6.247085	-3.581439	1.508863
H	-6.402594	-4.396570	2.231993
C	-7.131890	-1.990455	-0.097025
H	-7.982927	-1.560804	-0.647235
C	2.639574	2.653413	0.632303
C	2.877826	-0.960840	-0.447825
C	-2.425507	-2.394376	-0.507197
C	1.760332	-2.620864	-1.360255
C	3.859119	-1.926086	-0.885267
H	4.941848	-1.802974	-0.766355
C	-0.610862	-3.226042	-1.444045
C	-1.956869	1.706977	0.562879
C	-2.805954	-3.651197	-1.112948
H	-3.818430	-4.066967	-1.099365
C	-3.321979	1.963629	0.957300
H	-3.706119	2.946158	1.255516
C	-3.018175	-0.216838	0.442964
C	3.167099	-2.950992	-1.472427
H	3.554466	-3.867490	-1.928864
C	1.447153	3.364618	0.697273
C	-3.974718	0.760528	0.922278
H	-5.015032	0.540229	1.180981
C	-0.969242	2.681276	0.586822
H	-1.259694	3.708544	0.834419
C	-3.346919	-1.541140	0.119257
N	0.913917	1.146222	0.202448
C	4.018710	3.139063	0.873932
C	1.307074	4.838168	0.851742
O	2.007985	5.660563	0.290300
O	0.280199	5.164508	1.686232
C	0.069253	6.576576	1.915633
H	-1.011757	6.666388	2.140948
H	0.297310	7.128722	0.981745
C	5.274185	4.894631	1.877121
H	5.838888	4.857209	0.923015
H	5.877305	4.344071	2.631711
C	0.923782	7.075517	3.069053
H	0.728573	6.489486	3.988960
H	0.695546	8.140041	3.278774
H	1.999552	6.995428	2.820403
C	4.966619	6.313431	2.313282
H	4.341367	6.819817	1.551956
H	5.906609	6.885864	2.442473
H	4.420161	6.325777	3.277538

Conformation 3.
Multiplicity: 2
Charge: 0
E(B97-3c) = -3367.156200049537 Hartree
E(M06/def2-TZVP) = -3366.987783231865 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3365.964460512888 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3366.029998563644 Hartree
E(PBEh-3c) = -3362.573107430876 Hartree
E(PM6) = 68.26084 Kcal/mol
E(PM7) = 113.73731 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3368.995951689086 Hartree
E(GFN1-xTB) = -130.532667801393 Hartree
E(GFN2-xTB) = -127.368916359100 Hartree
E(GFN-FF) = -15.776054394029 Hartree

Coordinates:

Co	0.194843	-0.280317	-0.073901
N	1.349045	1.137849	0.630146
O	-4.152780	4.409292	1.421693
O	-2.657441	3.949513	3.067284
C	-2.717278	0.539068	0.010474
C	3.564754	0.380850	-0.183752
N	-0.947487	-1.731738	-0.740020
C	-0.348073	2.572008	1.710517
H	-0.521376	3.450836	2.342341
C	-1.461245	1.929738	1.173128
C	3.957191	-1.866188	-1.229844
H	5.023409	-1.736013	-1.439166
C	5.009650	0.729480	-0.317856
N	1.786909	-1.309898	-0.582374
C	5.402717	1.827916	-1.112342
H	4.631615	2.408042	-1.641370
C	7.358551	0.338668	0.236017
H	8.121755	-0.243547	0.774595
C	6.005172	-0.008810	0.357847
H	5.705219	-0.854588	0.994612
C	6.756522	2.173349	-1.235217
H	7.046326	3.028847	-1.864193
C	1.003365	-4.903074	-1.576767
C	7.738456	1.429339	-0.562200
H	8.800591	1.701280	-0.657691
C	0.618761	-5.401715	-2.840162
H	0.118779	-4.728578	-3.552662
C	1.541440	-7.585608	-2.292743
H	1.750130	-8.629593	-2.571538
C	1.668180	-5.768370	-0.681084
H	1.971963	-5.385127	0.304714
C	1.932992	-7.099218	-1.035428
H	2.446585	-7.761963	-0.322356
C	0.885716	-6.732346	-3.194409
H	0.585244	-7.103365	-4.186179
C	-2.818874	2.424984	1.269609
C	0.959894	2.208512	1.423451
C	1.836069	-2.622289	-1.030706
C	2.720974	1.272756	0.495217
C	2.102803	2.995865	1.822323
H	2.050102	3.884019	2.462815
C	3.096732	-0.850116	-0.665890
C	-2.323213	-1.694752	-0.915096
C	3.181319	-2.977501	-1.424515
H	3.473492	-3.949299	-1.834821
C	-2.822658	-2.977769	-1.350269
H	-3.878524	-3.197779	-1.546566
C	-0.578830	-3.026234	-1.075723
C	3.197799	2.429254	1.226092
H	4.246089	2.739674	1.281911
C	-3.603373	1.563841	0.517455
C	-1.744412	-3.819665	-1.410444
H	-1.721614	-4.882111	-1.671979
C	-3.149771	-0.614904	-0.638580
H	-4.217051	-0.698994	-0.875700
C	0.740922	-3.485942	-1.190300
N	-1.410545	0.782231	0.399276
C	-3.296527	3.685209	1.895448
C	-5.083209	1.629980	0.404975
O	-5.827303	1.946588	1.314626
O	-5.510400	1.288193	-0.842593
C	-6.934781	1.405419	-1.068389
H	-7.470204	1.055403	-0.162628
H	-7.142508	0.714697	-1.908935
C	-3.065851	5.162375	3.735527
H	-4.162987	5.122690	3.900704
H	-2.878216	6.025634	3.061746
C	-7.314953	2.838146	-1.405465
H	-7.092867	3.507214	-0.551580
H	-8.399614	2.902624	-1.626020
H	-6.756422	3.197494	-2.292314
C	-2.291281	5.262186	5.033277
H	-2.487868	4.384520	5.680180
H	-2.592845	6.174323	5.585311
H	-1.199696	5.317507	4.848450

Conformation 32.
Multiplicity: 2
Charge: 0
E(B97-3c) = -3367.153712380089 Hartree
E(M06/def2-TZVP) = -3366.984177544703 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3365.961902676208 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3366.027311552042 Hartree
E(PBEh-3c) = -3362.571252763582 Hartree
E(PM6) = 71.05000 Kcal/mol
E(PM7) = 116.59040 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3368.990966907922 Hartree
E(GFN1-xTB) = -130.527860062174 Hartree
E(GFN2-xTB) = -127.364912983311 Hartree
E(GFN-FF) = -15.769901516953 Hartree

Coordinates:

Co	-0.122564	-0.369242	0.189884
N	-1.877384	-0.032880	-0.630422
O	-1.788608	5.429839	-0.313928
O	0.338059	6.198859	-0.050214
C	1.467154	2.187713	0.459883
C	-2.598935	-2.343740	-1.149505
N	1.628222	-0.717769	1.013939
C	-1.946107	2.436805	-0.491640
H	-2.538025	3.345224	-0.661635
C	-0.629733	2.604021	-0.072701
C	-1.532105	-4.361851	-0.125772
H	-2.276170	-5.085261	-0.473950
C	-3.610841	-3.220994	-1.808354
N	-0.495262	-2.296494	0.183507
C	-4.944599	-3.271643	-1.348948
H	-5.238572	-2.655128	-0.486146
C	-4.177515	-4.872148	-3.520290
H	-3.872088	-5.496223	-4.373989
C	-3.238531	-4.035588	-2.899290
H	-2.199882	-4.001578	-3.261439
C	-5.882542	-4.109793	-1.969611

H	-6.917041	-4.142021	-1.594967
C	2.049475	-4.305975	2.208220
C	-5.502559	-4.910861	-3.058171
H	-6.239154	-5.567951	-3.544898
C	2.199715	-4.323447	3.611463
H	1.831165	-3.469359	4.199478
C	3.268360	-6.506007	3.499726
H	3.742317	-7.362663	4.002471
C	2.524973	-5.405394	1.461443
H	2.426602	-5.390986	0.365551
C	3.129249	-6.496675	2.102715
H	3.499955	-7.343578	1.505286
C	2.802741	-5.415950	4.251925
H	2.906458	-5.416606	5.347708
C	0.034631	3.891022	0.031141
C	-2.490043	1.199256	-0.809012
C	0.201652	-3.295187	0.855880
C	-2.750484	-0.951281	-1.195121
C	-3.755687	1.052515	-1.488927
H	-4.418964	1.886649	-1.745714
C	-1.556956	-2.947964	-0.428250
C	2.673671	0.183000	1.175431
C	-0.459097	-4.571652	0.698022
H	-0.131134	-5.506421	1.162912
C	3.815884	-0.454120	1.786291
H	4.763518	0.051226	2.006351
C	2.100886	-1.907763	1.542700
C	-3.901075	-0.280307	-1.766326
H	-4.715004	-0.782496	-2.298443
C	1.363190	3.620885	0.332972
C	3.455230	-1.751642	2.033356
H	4.047748	-2.552668	2.486757
C	2.624307	1.537533	0.880817
H	3.515280	2.145076	1.088438
C	1.417311	-3.133091	1.534986
N	0.254010	1.574036	0.188803
C	-0.598542	5.212010	-0.130668
C	2.501659	4.555775	0.614538
O	2.904498	4.752895	1.743085
O	3.127608	5.130999	-0.438340
C	2.708035	4.851656	-1.789318
H	1.699010	5.283452	-1.951807
H	2.635453	3.752622	-1.939367
C	-0.138044	7.560799	-0.086329
H	-0.981403	7.623790	-0.803592
H	0.720339	8.143445	-0.473805
C	3.729515	5.468636	-2.724008
H	3.794424	6.563602	-2.568107
H	3.442425	5.282646	-3.777934
H	4.735177	5.036208	-2.553425
C	-0.556689	8.031327	1.296887
H	-1.434382	7.458474	1.654233
H	-0.835461	9.103983	1.265103
H	0.271272	7.906419	2.022458
C	7.255461	0.709407	2.044659
H	7.858296	1.629669	2.079106
C	-0.635081	2.717026	4.080621
C	7.826073	-0.520444	2.408982
H	8.876331	-0.568071	2.734445
C	0.096330	3.858648	4.474641
H	0.943475	4.191383	3.856301
C	-1.350275	4.156345	6.407629
H	-1.628187	4.715794	7.313733
C	-1.734586	2.312397	4.867965
H	-2.309205	1.423207	4.567506
C	-2.087501	3.025180	6.023307
H	-2.943231	2.691503	6.629860
C	-0.258616	4.571939	5.628737
H	0.318360	5.463481	5.918236
C	-1.355089	-1.909088	-3.235864
C	2.013241	-1.947909	-1.536676
C	0.976259	1.327939	2.759405
C	3.287216	-0.988462	-0.022209
C	3.347392	-2.461742	-1.736613
H	3.621547	-3.189344	-2.509407
C	2.792799	0.372112	1.953252
C	-2.120536	1.583431	-0.179322
C	1.983288	1.403592	3.794339
H	1.830018	1.845255	4.783773
C	-2.935988	2.568989	0.491324
H	-3.850234	3.005389	0.072341
C	-1.167939	1.968919	1.766260
C	4.149434	-1.839152	-0.818044
H	5.228210	-1.947527	-0.668865
C	-2.296868	-0.904691	-3.046836
C	-2.356514	2.795112	1.711488
H	-2.680360	3.470508	2.509814
C	-2.493381	0.983157	-1.374738
H	-3.412713	1.320318	-1.865119
C	-0.272811	1.961286	2.846044
N	-0.610271	-0.586106	-1.465785
C	-1.255946	-2.967524	-4.297549
C	-3.506855	-0.788810	-3.881575
O	-3.831911	-1.633290	-4.707572
O	-4.227056	0.340948	-3.656723
C	-5.406807	0.521224	-4.474390
H	-6.055269	1.191933	-3.877444
H	-5.908306	-0.459953	-4.595687
C	-2.984075	-4.287199	-3.159646
H	-3.122144	-3.358786	-2.570259
H	-2.565971	-5.060926	-2.479340
C	-5.062463	1.126496	-5.825117
H	-4.516445	2.083193	-5.704903
H	-5.991096	1.326491	-6.396915
H	-4.438021	0.429104	-6.416020
C	-4.288490	-4.746382	-3.783987
H	-4.691580	-3.950952	-4.438879
H	-5.030704	-4.971622	-2.991567
H	-4.134942	-5.663210	-4.386727

Conformation 34.
Multiplicity: 2
Charge: 0
E(B97-3c) = converged!) Hartree
E(M06/def2-TZVP) = -3366.980438631788 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3365.958970872829 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3366.023597447263 Hartree
E(PBEh-3c) = -3362.566554723307 Hartree
E(PM6) = 73.79551 Kcal/mol
E(PM7) = 105.72296 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3368.986691458641 Hartree
E(GFN1-xTB) = -130.525908425129 Hartree
E(GFN2-xTB) = -127.361609999001 Hartree
E(GFN-FF) = -15.767266564779 Hartree

Coordinates:

Co	0.456405	0.070127	0.070517
N	1.984542	-1.028473	-0.496935
O	-0.438382	-2.865773	-5.192071
O	-2.012054	-4.079357	-4.202022
C	-1.817331	-0.097889	-1.934763
C	3.702315	-0.319341	1.138175
N	-1.020384	1.243376	0.594766
C	0.930639	-2.312123	-2.323452
H	1.084868	-3.077679	-3.095144
C	-0.297935	-1.657618	-2.287332
C	3.120146	0.837603	3.282104
H	4.094634	0.709903	3.764053
C	5.128125	-0.399012	1.570087
N	1.466981	0.649969	1.648966
C	5.916829	0.770340	1.631026
H	5.468366	1.732663	1.341560
C	7.049441	-1.689004	2.358871
H	7.486792	-2.655492	2.652363
C	5.711444	-1.629554	1.942686
H	5.098297	-2.542847	1.916557

Conformation 7.
Multiplicity: 2
Charge: 0
E(B97-3c) = -3367.153670342082 Hartree
E(M06/def2-TZVP) = -3366.984857878342 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3365.961870035470 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3366.027239527120 Hartree
E(PBEh-3c) = -3362.571294220884 Hartree
E(PM6) = 71.42599 Kcal/mol
E(PM7) = 116.51352 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3368.990213927448 Hartree
E(GFN1-xTB) = -130.527586939730 Hartree
E(GFN2-xTB) = -127.364617110551 Hartree
E(GFN-FF) = -15.768817979146 Hartree

Coordinates:

Co	0.400552	-0.228915	-0.264917
N	-0.959671	-1.457417	-0.982371
O	-2.530867	-2.954505	4.383151
O	-4.019901	-1.304826	4.273840
C	-0.169153	0.468378	2.626349
C	-0.452600	-1.344767	-3.403847
N	1.757504	1.002164	0.436007
C	-2.080851	-2.120614	1.116262
H	-2.834015	-2.777874	1.571325
C	-1.426632	-1.203269	1.935292
C	1.703981	-0.448136	-4.299980
H	1.557179	-0.779649	-5.332770
C	-0.859002	-1.733986	-4.786318
N	1.240240	-0.132805	-2.036424
C	-0.863505	-3.085423	-5.194172
H	-0.556201	-3.862075	-4.477796
C	-1.606006	-1.095153	-7.024975
H	-1.898967	-0.310389	-7.739012

C	-1.230539	-0.743039	-5.720283
H	-1.227877	0.312526	-5.409063
C	-1.237602	-3.436429	-6.499594
H	-1.229906	-4.494392	-6.803214
C	4.651099	1.591013	-1.963142
C	-1.612082	-2.442827	-7.418138
H	-1.905945	-2.718931	-8.442161
C	5.841574	1.093823	-1.390583
H	5.777063	0.332316	-0.598698
C	7.172244	2.522290	-2.842002
H	8.153462	2.884111	-3.184811
C	4.743541	2.567528	-2.978220
H	3.819637	2.973440	-3.416968
C	5.994396	3.028720	-3.414093
H	6.048770	3.794592	-4.202794
C	7.091975	1.554531	-1.828249
H	8.010720	1.151427	-1.375588
C	-1.792917	-0.969154	3.310354
C	-1.895654	-2.183619	-0.257388
C	2.492576	0.381769	-2.350829
C	-1.225299	-1.759861	-2.309394
C	-2.751579	-2.945808	-1.135124
H	-3.569448	-3.592490	-0.796311
C	0.746659	-0.636804	-3.232679
C	1.740377	1.652171	1.662543
C	2.801364	0.153232	-3.744983
H	3.743860	0.427827	-4.228529
C	2.884888	2.522074	1.800773
H	3.082054	3.148135	2.678707
C	2.920228	1.434673	-0.181405
C	-2.363452	-2.650709	-2.414641
H	-2.791611	-3.007284	-3.356553
C	-1.014682	0.095767	3.746691
C	3.632937	2.371425	0.664001
H	4.574386	2.859728	0.392751
C	0.823869	1.441325	2.683712
H	0.923240	2.001806	3.621966
C	3.326562	1.100213	-1.481279
N	-0.439386	-0.322478	1.524877
C	-2.786560	-1.816653	4.046501
C	-1.005643	0.713371	5.085223
O	-0.305534	1.648864	5.449870
O	-1.910381	0.097924	5.896879
C	-2.042127	0.610095	7.238548
H	-1.042470	0.929182	7.596181
H	-2.386698	-0.256674	7.835027
C	-4.378002	0.005123	3.791284
H	-4.228511	0.050706	2.690433
H	-3.716458	0.764692	4.254824
C	-3.032727	1.762179	7.296644
H	-2.666427	2.621982	6.702241
H	-3.161332	2.100741	8.344530
H	-4.025785	1.454975	6.910872
C	-5.826690	0.248751	4.164763
H	-6.488473	-0.516434	3.713415
H	-6.150007	1.246970	3.808764
H	-5.957761	0.210828	5.264699
H	-5.589749	-1.640392	-5.754567
C	-4.360474	-1.137307	-4.038685
H	-3.463781	-0.931054	-4.642340
C	-6.651746	-1.621813	-2.496151
H	-7.547672	-1.813050	-1.886014
C	-2.161052	4.851878	0.637941
C	-6.703312	-1.776380	-3.890510
H	-7.640124	-2.085321	-4.378499
C	-1.458603	5.976837	0.155011
H	-0.517206	5.823991	-0.394041
C	-3.157309	7.464252	1.060219
H	-3.545365	8.480936	1.224448
C	-3.367764	5.056693	1.340842
H	-3.912348	4.185744	1.735562
C	-3.861676	6.352747	1.549703
H	-4.801241	6.495451	2.105054
C	-1.954058	7.272399	0.363008
H	-1.396636	8.138422	-0.025258
C	3.356087	-1.880394	0.149587
C	0.151345	-2.135327	-1.823169
C	-2.318463	2.570026	-0.381173
C	-1.908211	-1.384318	-2.002035
C	-0.557831	-3.075126	-2.658295
H	-0.112416	-3.977636	-3.093111
C	-2.991104	0.724886	-1.382837
C	1.279730	1.973184	1.852620
C	-3.606700	2.859839	-0.970336
H	-4.109072	3.830976	-0.924921
C	1.251653	3.214962	2.589098
H	1.974617	3.487591	3.366678
C	-0.438377	3.114463	1.090845
C	-1.850275	-2.630191	-2.739356
H	-2.697946	-3.086687	-3.259769
C	3.568160	-0.964891	1.170443
C	0.194744	3.936341	2.102609
H	-0.154717	4.929145	2.403566
C	2.295690	1.037382	1.989420
H	3.095537	1.212483	2.720475
C	-1.615781	3.479172	0.423021
N	1.515924	-0.448089	0.189523
C	4.258319	-2.958003	-0.375920
C	4.734679	-0.884035	2.068875
O	4.994660	0.017972	2.852028
O	5.518261	-1.986305	1.916778
C	6.740304	-2.031644	2.678559
H	6.504556	-1.849232	3.748270
H	7.395102	-1.197095	2.347956
C	3.380421	-4.385755	1.381811
H	2.321143	-4.182869	1.111781
H	3.670055	-3.677385	2.184493
C	7.376490	-3.386090	2.441797
H	6.720533	-4.203685	2.802529
H	8.340948	-3.452430	2.982864
H	7.566273	-3.549799	1.362790
C	3.571725	-5.823446	1.821890
H	3.296590	-6.526942	1.011465
H	2.937229	-6.040049	2.704002
H	4.628775	-6.012014	2.096522

Conformation 8.
Multiplicity: 2
Charge: 0
E(B97-3c) = -3367.154119375566 Hartree
E(M06/def2-TZVP) = -3366.985739053207 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3365.962259767386 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -3366.027980937023 Hartree
E(PBEh-3c) = -3362.572047966654 Hartree
E(PM6) = 72.23415 Kcal/mol
E(PM7) = 116.67385 Kcal/mol
E(ωB97X-V/def2-TZVP) = -3368.991576301752 Hartree
E(GFN1-xTB) = -130.526583704417 Hartree
E(GFN2-xTB) = -127.364666652091 Hartree
E(GFN-FF) = -15.768569036261 Hartree

Coordinates:

Co	-0.217741	0.406859	-0.238094
N	-0.681461	-1.099115	-1.420832
O	4.963679	-2.785479	-1.347956
O	4.223327	-4.167893	0.231610
C	2.422518	-0.073979	1.163685
C	-3.034765	-0.550293	-1.965944
N	0.229330	1.908412	0.947436
C	1.465009	-2.322431	-1.416202
H	2.023251	-3.169828	-1.837340
C	2.079808	-1.549689	-0.434597
C	-4.038487	1.705101	-1.565093
H	-4.966210	1.528037	-2.118214
C	-4.295954	-0.983148	-2.637040
N	-1.932913	1.264476	-0.663090
C	-5.458304	-1.226503	-1.874289
H	-5.414855	-1.106416	-0.781253
C	-5.554784	-1.531071	-4.659874

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Conformation 15.
Multiplicity: 2Charge: 0
E(B97-3c) = -2948.798826903968 Hartree
E(M06/def2-TZVP) = -2948.910938074289 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -2947.690999370790 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -2947.965475922643 Hartree
E(PBEh-3c) = -2944.948574562258 Hartree
E(PM6) = -240.82987 Kcal/mol
E(PM7) = -237.54253 Kcal/mol
E(ωB97X-V/def2-TZVP) = -2949.536671886141 Hartree
E(GFN1-xTB) = -184.761142349843 Hartree
E(GFN2-xTB) = -119.355662246845 Hartree
E(GFN-FF) = -16.235874247916 Hartree

Coordinates:

Ti	-0.249646	0.084504	0.330300
Si	-2.589284	-1.741210	2.160932
Si	-1.869116	1.344554	2.851139
O	1.088659	-1.166865	0.369543
O	-0.608686	1.368743	-0.923206
C	-1.870596	-0.081500	1.597721
H	-2.584681	0.271314	0.806976
C	2.190835	-1.937049	0.202094
C	3.066473	-2.128318	1.320159
C	4.214227	-2.918016	1.121607
H	4.908695	-3.080191	1.954916
C	4.501742	-3.502719	-0.114222
H	5.408190	-4.113213	-0.239942
C	3.630435	-3.309910	-1.189050

H	3.871768	-3.779144	-2.150795
C	2.460663	-2.534569	-1.073157
C	2.791324	-1.502470	2.706419
C	3.868660	-1.896699	3.737898
H	3.921258	-2.993843	3.885548
H	3.616088	-1.440441	4.716031
H	4.876558	-1.533218	3.453147
C	2.807556	0.040522	2.615161
H	3.753685	0.399782	2.162840
H	2.720559	0.486169	3.627622
H	1.970853	0.430090	2.004676
C	1.436381	-1.997178	3.261166
H	0.590871	-1.703410	2.614985
H	1.256198	-1.569457	4.268689
H	1.430517	-3.102263	3.350351
C	1.523314	-2.376674	-2.292953
C	2.019228	-3.181245	-3.512112
H	3.012531	-2.840477	-3.867735
H	1.305041	-3.043453	-4.348750
H	2.077459	-4.267635	-3.299934
C	1.449354	-0.900136	-2.737741
H	1.048923	-0.238173	-1.949968
H	0.783912	-0.791528	-3.618220
H	2.452161	-0.519980	-3.017497
C	0.115470	-2.909335	-1.950253
H	0.162307	-3.969430	-1.630278
H	-0.549458	-2.843212	-2.835604
H	-0.351137	-2.334373	-1.130807
C	-0.526898	2.038195	-2.095447
C	-1.626843	1.934616	-3.014060
C	-1.521558	2.616748	-4.237519
H	-2.337570	2.551230	-4.968019
C	-0.398791	3.390736	-4.553272
H	-0.343242	3.919345	-5.516474
C	0.646795	3.491017	-3.636752
H	1.512243	4.119300	-3.891685
C	0.630847	2.818094	-2.396138
C	-2.900782	1.123339	-2.682538
C	-3.574336	1.706251	-1.417724
H	-4.456426	1.095661	-1.131700
H	-3.921383	2.742269	-1.605839
H	-2.877439	1.733422	-0.561751
C	-2.566252	-0.372408	-2.485183
H	-1.890142	-0.547419	-1.626034
H	-2.072503	-0.787359	-3.386328
H	-3.492409	-0.955659	-2.302059
C	-3.938593	1.195587	-3.821070
H	-4.838048	0.616407	-3.530972
H	-3.555212	0.760383	-4.765873
H	-4.263774	2.235701	-4.023290
C	1.848831	3.073969	-1.467306
C	3.161801	2.868708	-2.263184
H	3.232675	1.828177	-2.639333
H	4.034725	3.055234	-1.604759
H	3.253770	3.548643	-3.131168
C	1.760095	4.538985	-0.975417
H	1.749295	5.253553	-1.821800
H	2.626580	4.786222	-0.327269
H	0.833175	4.697074	-0.387647
C	1.976311	2.178447	-0.220629
H	1.155772	2.340232	0.504495
H	2.918771	2.427485	0.307726
H	2.045673	1.103120	-0.482143
C	-1.902705	-3.199942	1.159474
H	-2.146736	-3.093416	0.082920
H	-2.355301	-4.150033	1.513343
H	-0.801771	-3.291017	1.250209
C	-2.291189	-2.117339	3.997943
H	-1.212140	-2.177984	4.240822
H	-2.748309	-3.098544	4.243275
H	-2.751466	-1.358248	4.661701
C	-4.465466	-1.686794	1.856244
H	-4.944265	-0.872517	2.436681
H	-4.948279	-2.644422	2.142782
H	-4.680289	-1.506774	0.781734
C	-3.593062	1.553739	3.625474
H	-4.354600	1.756372	2.844678
H	-3.596121	2.408393	4.333649
H	-3.910446	0.649597	4.182476
C	-1.460691	3.001242	2.004193
H	-0.400624	3.065935	1.684163
H	-1.640725	3.832568	2.717881
H	-2.091870	3.178342	1.109937
C	-0.605425	1.078232	4.236954
H	-0.807076	0.149966	4.805436
H	-0.639469	1.930424	4.947053
H	0.423615	1.011717	3.832402

Conformation 18.
Multiplicity: 2
Charge: 0

E(B97-3c) = -2948.799008603179 Hartree
E(M06/def2-TZVP) = -2948.911594541606 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -2947.691071045034 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -2947.965841782781 Hartree
E(PBEh-3c) = -2944.948731135618 Hartree
E(PM6) = -242.13411 Kcal/mol
E(PM7) = -237.72387 Kcal/mol
E(ωB97X-V/def2-TZVP) = -2949.536955821065 Hartree
E(GFN1-xTB) = -185.525070356678 Hartree
E(GFN2-xTB) = -119.357568975882 Hartree
E(GFN-FF) = -16.238101160526 Hartree

Coordinates:

Ti	-0.193762	-0.234261	-0.368563
Si	-2.907316	-2.436706	-0.123707
Si	-1.433031	-1.633432	-2.915310
O	-1.050667	1.155490	0.461925
O	1.584841	-0.694562	-0.388553
C	-1.367854	-1.806721	-1.022805
H	-0.588973	-2.593033	-0.858280
C	-1.262913	2.295643	1.163941
C	-1.883367	3.407537	0.505737
C	-2.034687	4.594832	1.246500
H	-2.494969	5.471375	0.774512
C	-1.620472	4.694043	2.577319
H	-1.751032	5.637476	3.128151
C	-1.055030	3.584419	3.210060
H	-0.754977	3.676278	4.261112
C	-0.861729	2.362484	2.538323
C	-2.418188	3.330528	-0.943770
C	-3.087473	4.649712	-1.379161
H	-3.950570	4.914413	-0.736162
H	-3.467310	4.537941	-2.414518
H	-2.377170	5.500855	-1.377028
C	-1.281289	3.057528	-1.952131
H	-0.501936	3.843128	-1.894173
H	-1.682304	3.046226	-2.986906
H	-0.793626	2.081140	-1.773287
C	-3.487054	2.221070	-1.038742
H	-3.063923	1.229720	-0.804947
H	-3.915040	2.186402	-2.062217
H	-4.317266	2.410817	-0.329085
C	-0.235305	1.163411	3.288336
C	-0.033959	1.463788	4.787950
H	0.677737	2.295931	4.958771
H	0.386015	0.565370	5.282993
H	-0.988636	1.709986	5.294348
C	1.162076	0.848493	2.710778
H	1.139953	0.591229	1.636026
H	1.623242	-0.013469	3.234739
H	1.837551	1.719868	2.823874
C	-1.160693	-0.072165	3.208542
H	-2.149243	0.151269	3.658123
H	-0.714705	-0.923547	3.763055
H	-1.334888	-0.400412	2.167673
C	2.887461	-0.783381	-0.030668
C	3.364303	-2.037216	0.486772
C	4.710221	-2.120587	0.877781
H	5.100052	-3.062896	1.282083
C	5.577064	-1.028289	0.762668
H	6.628583	-1.118533	1.073366
C	5.098451	0.172008	0.241529
H	5.796509	1.015225	0.139899
C	3.757267	0.342365	-0.165653
C	2.443903	-3.269629	0.612987
C	3.194998	-4.501566	1.157979
H	2.494518	-5.359274	1.209713
H	3.587132	-4.333183	2.180996
H	4.039560	-4.801489	0.505687
C	1.903272	-3.660638	-0.783563
H	2.733318	-4.007484	-1.431518
H	1.415927	-2.810572	-1.291311
H	1.167875	-4.487823	-0.699284
C	1.301534	-2.982541	1.614270
H	0.649826	-3.872683	1.723719
H	0.658065	-2.134869	1.309613
H	1.718419	-2.739461	2.612615
C	3.415385	1.725354	-0.782298
C	3.869124	2.850542	0.179845
H	3.334045	2.778763	1.148211
H	3.639550	3.841199	-0.263315
H	4.955204	2.825849	0.389601
C	4.185704	1.844825	-2.120122
H	5.278448	1.734016	-1.977372
H	4.000029	2.833870	-2.588829
H	3.858061	1.059914	-2.831748
C	1.933432	2.000162	-1.087299
H	1.522008	1.304739	-1.842804
H	1.837165	3.022390	-1.505212
H	1.307133	1.981510	-0.173476
C	-2.373602	-3.326228	1.465368

H	-1.722004	-4.193463	1.232421
H	-3.265441	-3.709506	2.003585
H	-1.818457	-2.660570	2.154568
C	-4.120327	-1.055799	0.332238
H	-3.645715	-0.284761	0.971521
H	-4.977521	-1.485291	0.891362
H	-4.523893	-0.549884	-0.567168
C	-3.871419	-3.726317	-1.140920
H	-4.259820	-3.316690	-2.095074
H	-4.741264	-4.089302	-0.554269
H	-3.236815	-4.603985	-1.380394
C	-1.283777	-3.345615	-3.720205
H	-0.345282	-3.841828	-3.396740
H	-1.259072	-3.256101	-4.826352
H	-2.130661	-4.003914	-3.444531
C	0.039909	-0.616753	-3.588655
H	-0.054106	0.467645	-3.370865
H	0.077553	-0.723221	-4.694324
H	1.013729	-0.966823	-3.187538
C	-3.016714	-0.768953	-3.488691
H	-3.926809	-1.315855	-3.170893
H	-3.033333	-0.695248	-4.595680
H	-3.078769	0.257754	-3.077069

Conformation 19.
Multiplicity: 2
Charge: 0
E(B97-3c) = -2948.800186434236 Hartree
E(M06/def2-TZVP) = -2948.912489165615 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -2947.691353850068 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -2947.966681188626 Hartree
E(PBEh-3c) = -2944.950971498311 Hartree
E(PM6) = -242.72091 Kcal/mol
E(PM7) = -239.10820 Kcal/mol
E(ωB97X-V/def2-TZVP) = -2950.750865069244 Hartree
E(GFN1-xTB) = -184.901846225052 Hartree
E(GFN2-xTB) = -119.360676620274 Hartree
E(GFN-FF) = -16.240378744308 Hartree

Coordinates:

Ti	-0.390808	-0.291344	-0.073004
Si	-0.568328	-3.592821	-0.890954
Si	-3.188564	-2.000989	0.124707
O	1.119519	-0.512770	0.926182
O	-0.809368	1.264090	-0.926158
C	-1.482006	-1.949682	-0.704704
H	-1.695555	-1.587326	-1.741613
C	2.176864	-0.322238	1.747527
C	1.986327	-0.380942	3.161136
C	3.125164	-0.189591	3.972201
H	3.017020	-0.243453	5.065365
C	4.386680	0.065707	3.436769
H	5.251035	0.216017	4.100715
C	4.544653	0.130791	2.047670
H	5.542359	0.336453	1.640648
C	3.464638	-0.061047	1.169700
C	0.659661	-0.673855	3.911861
C	-0.620754	-0.743085	3.058665
H	-0.824944	0.216169	2.539375
H	-1.486059	-0.936597	3.725598
H	-0.588576	-1.566620	2.319971
C	0.806330	-2.040872	4.623618
H	0.971407	-2.850925	3.884280
H	-0.112007	-2.279174	5.200007
H	1.661861	-2.046831	5.326976
C	0.413043	0.439576	4.959895
H	1.227896	0.513772	5.704595
H	-0.527558	0.239667	5.513588
H	0.316780	1.427543	4.464693
C	3.687545	-0.001470	-0.358748
C	5.169801	0.230347	-0.716652
H	5.549957	1.199219	-0.334909
H	5.275538	0.246946	-1.819891
H	5.823706	-0.578319	-0.333117
C	2.893118	1.168291	-0.983356
H	1.802389	1.077874	-0.831742
H	3.069132	1.211834	-2.077531
H	3.208181	2.136400	-0.546073
C	3.277725	-1.344039	-1.002979
H	3.881738	-2.177954	-0.591399
H	3.440274	-1.310674	-2.100289
H	2.214398	-1.578260	-0.822028
C	-0.730675	2.455129	-1.565689
C	-0.609404	3.660438	-0.802592
C	-0.468946	4.862829	-1.521744
H	-0.359905	5.808638	-0.976714
C	-0.459486	4.892665	-2.919053
H	-0.334511	5.848613	-3.449548
C	-0.623102	3.706608	-3.640493
H	-0.633672	3.753651	-4.736621
C	-0.775082	2.464852	-2.997011
C	-0.639851	3.684820	0.744341
C	-1.932203	3.020552	1.268756
H	-1.956947	3.055807	2.377812
H	-2.012308	1.964143	0.958923
H	-2.829171	3.549820	0.888301
C	-0.628827	5.126371	1.293967
H	-1.493545	5.716783	0.930164
H	0.300728	5.670960	1.033278
H	-0.689421	5.092798	2.400357
C	0.601829	2.974723	1.326466
H	0.587520	3.018852	2.435342
H	1.536340	3.456649	0.977269
H	0.657348	1.909252	1.042872
C	-1.005403	1.178938	-3.823541
C	0.162964	0.182827	-3.635285
H	1.119759	0.642188	-3.955594
H	-0.003562	-0.727861	-4.246766
H	0.291031	-0.146231	-2.584862
C	-2.361210	0.547879	-3.422361
H	-2.422303	0.346604	-2.338753
H	-2.520485	-0.408644	-3.963103
H	-3.194117	1.230595	-3.685512
C	-1.084682	1.473421	-5.335734
H	-1.904561	2.177743	-5.581017
H	-1.283635	0.528383	-5.880281
H	-0.136485	1.889053	-5.732196
C	0.564035	-3.497461	-2.412238
H	-0.047659	-3.358579	-3.328370
H	1.138975	-4.439555	-2.531426
H	1.287357	-2.661568	-2.360049
C	0.436084	-3.975957	0.672411
H	1.168046	-3.173065	0.892942
H	0.990882	-4.929960	0.559364
H	-0.233214	-4.078247	1.551473
C	-1.720921	-5.070663	-1.227408
H	-2.442061	-5.259560	-0.407963
H	-1.114765	-5.991295	-1.360395
H	-2.300199	-4.913283	-2.160290
C	-3.235178	-3.145422	1.637879
H	-3.024704	-4.199827	1.371756
H	-4.246514	-3.109275	2.093178
H	-2.506689	-2.838179	2.413529
C	-4.488608	-2.577730	-1.133646
H	-4.509797	-1.900594	-2.012864
H	-5.501523	-2.574338	-0.679045
H	-4.278375	-3.602488	-1.498609
C	-3.746425	-0.278051	0.714516
H	-3.150237	0.086795	1.575709
H	-4.805580	-0.323329	1.045960
H	-3.682389	0.480094	-0.092876

Conformation 27.
Multiplicity: 2
Charge: 0
E(B97-3c) = -2948.803891329012 Hartree
E(M06/def2-TZVP) = -2948.915175095847 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -2947.695438774124 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -2947.969672993215 Hartree
E(PBEh-3c) = -2944.952955564924 Hartree
E(PM6) = -241.69681 Kcal/mol
E(PM7) = -239.68146 Kcal/mol
E(ωB97X-V/def2-TZVP) = -2950.752305316419 Hartree
E(GFN1-xTB) = -184.829154260005 Hartree
E(GFN2-xTB) = -119.364115948828 Hartree
E(GFN-FF) = -16.239977096284 Hartree

Coordinates:

Ti	-0.446714	-0.113517	0.145374
Si	-3.299243	1.362745	1.370323
Si	-3.203310	-1.756519	0.509448
O	-0.201063	1.121250	-1.183512
O	0.821936	-1.181061	0.928959
C	-2.279305	-0.209168	1.108601
H	-1.890764	-0.503904	2.115017
C	0.493825	1.757680	-2.164881
C	0.251433	1.393883	-3.527856
C	1.024215	2.034615	-4.515153
H	0.871435	1.777907	-5.570548
C	1.989737	2.991739	-4.192130
H	2.584700	3.466119	-4.986672
C	2.181123	3.356999	-2.857023
H	2.928400	4.126224	-2.626825
C	1.439972	2.774024	-1.811179
C	-0.822855	0.359735	-3.938900
C	-0.948650	0.241151	-5.471393
H	-1.232066	1.202852	-5.944231
H	-1.740448	-0.495774	-5.713371
H	-0.011213	-0.115983	-5.942236
C	-0.459270	-1.049150	-3.418689
H	0.508864	-1.375479	-3.847339
H	-1.234766	-1.784602	-3.717228

H	-0.372934	-1.088210	-2.314098
C	-2.206810	0.792353	-3.406104
H	-2.238800	0.837214	-2.304224
H	-2.985221	0.079349	-3.748850
H	-2.474783	1.797163	-3.790261
C	1.676720	3.257627	-0.358394
C	2.634621	4.462607	-0.283992
H	3.651629	4.208311	-0.644021
H	2.729161	4.782583	0.772920
H	2.263292	5.330176	-0.865413
C	2.319042	2.125754	0.474073
H	1.663407	1.235566	0.528129
H	2.514594	2.461398	1.512933
H	3.277862	1.796518	0.028801
C	0.334370	3.706858	0.263759
H	-0.094629	4.548684	-0.316588
H	0.489589	4.054680	1.305950
H	-0.411754	2.894232	0.275769
C	1.997180	-1.598879	1.469763
C	2.132646	-1.498710	2.896554
C	3.371493	-1.863245	3.457723
H	3.518330	-1.786305	4.541783
C	4.427033	-2.334800	2.672384
H	5.384099	-2.613197	3.138587
C	4.254398	-2.473624	1.293606
H	5.082831	-2.867364	0.692175
C	3.050740	-2.120142	0.655849
C	0.979450	-1.050774	3.816768
C	1.373716	-1.118462	5.309804
H	0.505087	-0.814686	5.927674
H	2.208807	-0.432339	5.555521
H	1.660074	-2.143636	5.618725
C	-0.221106	-2.011583	3.640800
H	0.047433	-3.028465	3.986072
H	-0.541796	-2.091356	2.587760
H	-1.086067	-1.665021	4.244041
C	0.588999	0.421446	3.562094
H	-0.233644	0.729796	4.238727
H	0.233899	0.616024	2.530407
H	1.457442	1.086551	3.740146
C	2.902902	-2.312197	-0.873225
C	2.747705	-0.939292	-1.561975
H	1.835588	-0.405020	-1.246141
H	2.692118	-1.059097	-2.663062
H	3.611278	-0.284167	-1.333929
C	4.140634	-2.988550	-1.493566
H	5.054800	-2.370978	-1.384555
H	3.967095	-3.134124	-2.578716
H	4.337457	-3.984924	-1.049927
C	1.691147	-3.226376	-1.162314
H	1.861929	-4.238350	-0.742075
H	1.532720	-3.332739	-2.255379
H	0.762356	-2.832716	-0.714797
C	-3.493859	2.318534	-0.246928
H	-2.512474	2.616578	-0.664975
H	-4.098924	3.230210	-0.078000
H	-4.031162	1.727816	-1.017853
C	-5.033736	1.041796	2.082862
H	-5.666998	0.420826	1.417927
H	-5.554814	2.011627	2.228033
H	-4.974981	0.543118	3.072011
C	-2.414211	2.453863	2.647437
H	-2.354124	1.937232	3.627339
H	-2.972094	3.401042	2.801449
H	-1.383488	2.714103	2.337120
C	-4.395158	-1.367014	-0.911361
H	-5.168669	-0.629733	-0.617183
H	-4.914188	-2.292855	-1.234248
H	-3.850759	-0.956489	-1.785069
C	-4.153874	-2.531971	1.959670
H	-3.465980	-2.750991	2.802624
H	-4.623243	-3.488357	1.647965
H	-4.949493	-1.861369	2.339838
C	-2.030213	-3.125915	-0.105448
H	-1.497339	-2.879355	-1.051793
H	-2.622707	-4.045796	-0.299538
H	-1.261613	-3.384228	0.651870

Conformation 29.
Multiplicity: 2
Charge: 0
E(B97-3c) = -2948.791163204811 Hartree
E(M06/def2-TZVP) = -2948.905511797009 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -2947.683627294572 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -2947.958092797182 Hartree
E(PBEh-3c) = -2944.943985125730 Hartree
E(PM6) = -238.12200 Kcal/mol
E(PM7) = -233.41507 Kcal/mol
E(ωB97X-V/def2-TZVP) = -2949.529129626508 Hartree
E(GFN1-xTB) = -182.425733895070 Hartree
E(GFN2-xTB) = -119.352012362808 Hartree
E(GFN-FF) = -16.231355531878 Hartree

Coordinates:

Ti	-0.300105	-0.208153	0.134316
Si	-0.795552	-2.750629	2.316985
Si	-2.881174	-0.336303	2.315353
O	1.130723	0.616398	0.946917
O	-0.793835	-0.264188	-1.635990
C	-1.581653	-1.328620	1.338198
H	-2.150658	-1.817856	0.505937
C	2.233260	1.403534	1.071460
C	3.541053	0.824319	1.134940
C	4.637419	1.711667	1.196291
H	5.652839	1.295694	1.251833
C	4.486082	3.095984	1.204145
H	5.367831	3.752790	1.240956
C	3.198543	3.639968	1.191995
H	3.087871	4.730350	1.229641
C	2.052787	2.828676	1.142517
C	3.897909	-0.680989	1.259048
C	4.339073	-0.928427	2.723002
H	5.210802	-0.303182	3.000762
H	4.618099	-1.993259	2.868149
H	3.514508	-0.692294	3.425369
C	2.762664	-1.666257	0.948555
H	1.937237	-1.582164	1.671216
H	3.154235	-2.702268	1.012333
H	2.359076	-1.527196	-0.069358
C	5.063993	-1.042959	0.307188
H	4.791555	-0.841128	-0.748449
H	5.296195	-2.123626	0.397683
H	5.997014	-0.490161	0.526524
C	0.655918	3.485159	1.209887
C	0.741867	5.014819	1.394779
H	1.279335	5.292856	2.323170
H	-0.284312	5.427563	1.467612
H	1.238837	5.515608	0.539913
C	-0.111461	2.936058	2.435079
H	-0.250154	1.840805	2.387691
H	-1.111608	3.408805	2.512743
H	0.446010	3.163808	3.365841
C	-0.120332	3.255944	-0.103866
H	0.445497	3.648423	-0.972219
H	-1.106749	3.762195	-0.074504
H	-0.319849	2.183901	-0.304450
C	-0.933822	-0.280262	-2.988208
C	0.172140	-0.678885	-3.809476
C	-0.013403	-0.689938	-5.204338
H	0.816398	-0.990302	-5.855505
C	-1.228733	-0.332034	-5.790846
H	-1.344565	-0.351894	-6.884775
C	-2.296196	0.050450	-4.976279
H	-3.244600	0.329294	-5.451044
C	-2.189700	0.091184	-3.573278
C	1.529066	-1.116197	-3.220312
C	2.548456	-1.494417	-4.314928
H	3.499119	-1.797954	-3.832031
H	2.775939	-0.643947	-4.988382
H	2.204343	-2.347011	-4.933659
C	1.320360	-2.385134	-2.362433
H	0.893574	-3.197900	-2.983657
H	0.622150	-2.216345	-1.519398
H	2.282375	-2.743582	-1.944076
C	2.166305	0.046907	-2.426636
H	3.150530	-0.248633	-2.011891
H	1.548395	0.400052	-1.581227
H	2.326977	0.919029	-3.091307
C	-3.398756	0.556853	-2.734816
C	-4.629016	0.873814	-3.609182
H	-4.436193	1.699743	-4.322631
H	-5.464123	1.192417	-2.953464
H	-4.975007	-0.009445	-4.182680
C	-3.828636	-0.553395	-1.750302
H	-4.114713	-1.470665	-2.303678
H	-4.707722	-0.227448	-1.156455
H	-3.020852	-0.818794	-1.047845
C	-3.024518	1.860496	-1.996708
H	-2.187583	1.709896	-1.293393
H	-3.889109	2.248394	-1.420423
H	-2.722970	2.639763	-2.725529
C	-2.082937	-3.820682	3.221646
H	-2.619746	-3.260734	4.013373
H	-1.572978	-4.680274	3.705737
H	-2.836961	-4.227523	2.517182
C	0.065975	-3.937705	1.108648
H	-0.683690	-4.385468	0.423097
H	0.555029	-4.767746	1.660210
H	0.835925	-3.443289	0.486956
C	0.410190	-2.095489	3.639321
H	0.815335	-1.098035	3.376761
H	1.265170	-2.788016	3.777293

H	-0.104215	-1.996916	4.615617
C	-3.333644	1.332946	1.529380
H	-2.457001	1.972752	1.315871
H	-3.996105	1.890660	2.224939
H	-3.888103	1.186253	0.583943
C	-2.288704	0.020252	4.082233
H	-2.191506	-0.900855	4.690300
H	-3.022595	0.681073	4.588417
H	-1.307912	0.537259	4.090362
C	-4.513891	-1.305357	2.372703
H	-4.878018	-1.498049	1.342031
H	-5.292090	-0.714041	2.899483
H	-4.414228	-2.280789	2.886093

Conformation 30.
Multiplicity: 2
Charge: 0
E(B97-3c) = -2948.802276506778 Hartree
E(M06/def2-TZVP) = -2948.914707507206 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -2947.694500312586 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -2947.969024251896 Hartree
E(PBEh-3c) = -2944.953222712317 Hartree
E(PM6) = -241.84948 Kcal/mol
E(PM7) = -239.71992 Kcal/mol
E(ωB97X-V/def2-TZVP) = -2949.540600975737 Hartree
E(GFN1-xTB) = -183.882366870867 Hartree
E(GFN2-xTB) = -119.363430066704 Hartree
E(GFN-FF) = -16.242713488232 Hartree

Coordinates:

Ti	0.250663	-0.096100	-0.354447
Si	3.181711	0.206908	-2.172044
Si	1.429299	-2.485404	-2.337591
O	0.886681	0.597109	1.206376
O	-1.522391	-0.287852	-0.719506
C	1.492161	-0.628305	-1.934626
H	0.824733	-0.146007	-2.699048
C	1.107429	1.081858	2.452651
C	1.841966	0.272177	3.378277
C	2.048657	0.791451	4.669752
H	2.604586	0.200737	5.407950
C	1.565865	2.047740	5.044468
H	1.744173	2.427622	6.061541
C	0.859367	2.821865	4.120856
H	0.493690	3.806688	4.435277
C	0.606191	2.375938	2.809405
C	2.393719	-1.124792	3.009099
C	3.199393	-1.745581	4.168657
H	4.072178	-1.123473	4.451519
H	3.584398	-2.735991	3.853408
H	2.577590	-1.904499	5.072237
C	1.233456	-2.098824	2.703960
H	0.551144	-2.179997	3.573361
H	1.629800	-3.110757	2.481022
H	0.629158	-1.777402	1.833654
C	3.350270	-1.029144	1.800435
H	2.837118	-0.673862	0.889760
H	3.782837	-2.025747	1.577145
H	4.185386	-0.331210	2.012070
C	-0.184292	3.279501	1.832086
C	0.650852	3.575227	0.567606
H	1.609293	4.064825	0.832958
H	0.092617	4.251469	-0.112120
H	0.893550	2.655724	0.005914
C	-0.528447	4.643738	2.465658
H	-1.183396	4.540356	3.353676
H	-1.075330	5.258170	1.722743
H	0.377924	5.208209	2.762808
C	-1.527234	2.617897	1.451687
H	-1.398624	1.666231	0.906820
H	-2.115723	3.292317	0.796875
H	-2.131346	2.406728	2.355967
C	-2.872140	-0.171741	-0.762807
C	-3.457415	0.633614	-1.793112
C	-4.858156	0.767489	-1.789361
H	-5.344943	1.384986	-2.554155
C	-5.656182	0.127750	-0.837185
H	-6.749359	0.250039	-0.860724
C	-5.062340	-0.676368	0.138964
H	-5.709821	-1.178517	0.867868
C	-3.667131	-0.852795	0.213710
C	-2.616246	1.310101	-2.901319
C	-3.498930	2.094578	-3.893422
H	-2.855762	2.535825	-4.680953
H	-4.043588	2.926358	-3.403024
H	-4.238957	1.441613	-4.397286
C	-1.876628	0.222806	-3.714218
H	-2.602981	-0.439247	-4.227158
H	-1.246942	-0.411721	-3.068598
H	-1.230830	0.688920	-4.487559
C	-1.611547	2.325276	-2.311368
H	-1.052980	2.829364	-3.126817
H	-0.862291	1.850212	-1.646994
H	-2.131909	3.102499	-1.717230
C	-3.061753	-1.733454	1.334006
C	-2.159425	-2.846807	0.755696
H	-2.723866	-3.487218	0.048351
H	-1.778875	-3.490274	1.575084
H	-1.282689	-2.442771	0.217106
C	-2.266090	-0.853520	2.323537
H	-1.396617	-0.359050	1.854284
H	-1.881647	-1.467663	3.162977
H	-2.911582	-0.058766	2.746561
C	-4.158925	-2.443917	2.154559
H	-4.816536	-1.728178	2.686845
H	-3.677908	-3.080981	2.923379
H	-4.793291	-3.099465	1.524784
C	3.360024	0.686849	-4.001863
H	3.331662	-0.203207	-4.661462
H	4.318803	1.217452	-4.179149
H	2.537128	1.364966	-4.310827
C	3.354766	1.808324	-1.167217
H	2.598925	2.560614	-1.471057
H	4.356567	2.252718	-1.345614
H	3.247689	1.638717	-0.077165
C	4.642290	-0.906808	-1.693309
H	4.616261	-1.183990	-0.621832
H	5.587871	-0.354547	-1.874133
H	4.679709	-1.839940	-2.288688
C	-0.348507	-3.066996	-2.667501
H	-1.054891	-2.808298	-1.856222
H	-0.355634	-4.170759	-2.786521
H	-0.740592	-2.627772	-3.607084
C	2.144702	-3.507666	-0.909562
H	3.191760	-3.224091	-0.685262
H	2.129304	-4.587656	-1.164759
H	1.551805	-3.367962	0.017011
C	2.381613	-2.909274	-3.930536
H	1.972767	-2.341602	-4.791678
H	2.265342	-3.990634	-4.153963
H	3.465845	-2.692951	-3.864323

Conformation 32.
Multiplicity: 2
Charge: 0
E(B97-3c) = -2948.795389771905 Hartree
E(M06/def2-TZVP) = -2948.907235114917 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -2947.687910692649 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -2947.962032391801 Hartree
E(PBEh-3c) = -2944.946301764185 Hartree
E(PM6) = -239.70165 Kcal/mol
E(PM7) = -237.61489 Kcal/mol
E(ωB97X-V/def2-TZVP) = -2950.746549455186 Hartree
E(GFN1-xTB) = -183.227376004867 Hartree
E(GFN2-xTB) = -119.356187457274 Hartree
E(GFN-FF) = -16.234881433313 Hartree

Coordinates:

Ti	0.356914	-0.081411	0.367559
Si	0.293980	-1.068460	3.592250
Si	3.018437	-1.484275	1.908412
O	-0.938803	-1.236036	-0.214424
O	0.758781	1.543663	-0.374777
C	1.373867	-0.557257	2.120995
H	1.709618	0.485621	2.347673
C	-1.884530	-1.743396	-1.048130
C	-1.570194	-2.906151	-1.823458
C	-2.532542	-3.344766	-2.752194
H	-2.320498	-4.221885	-3.375767
C	-3.759656	-2.694908	-2.905783
H	-4.487838	-3.055403	-3.647590
C	-4.068037	-1.600941	-2.093756
H	-5.049386	-1.124377	-2.206254
C	-3.160319	-1.099771	-1.141075
C	-0.250653	-3.692425	-1.651573
C	-0.229568	-4.973150	-2.510667
H	-1.060418	-5.659777	-2.252522
H	0.720308	-5.515151	-2.329609
H	-0.281938	-4.753715	-3.595891
C	0.961841	-2.843139	-2.088783
H	0.885547	-2.563544	-3.158175
H	1.903100	-3.414094	-1.949498
H	1.048733	-1.906614	-1.504764
C	-0.099043	-4.135008	-0.179516
H	-0.030752	-3.273440	0.506250
H	0.816043	-4.750915	-0.059849
H	-0.965663	-4.751069	0.134143
C	-3.579229	0.075809	-0.226477
C	-3.444309	-0.341430	1.254941
H	-4.100277	-1.206838	1.478140
H	-3.742591	0.494229	1.921263
H	-2.409549	-0.630389	1.509299

C	-5.054687	0.470850	-0.446444
H	-5.239677	0.853759	-1.470027
H	-5.321460	1.280614	0.261814
H	-5.743868	-0.376739	-0.260380
C	-2.742348	1.341441	-0.513914
H	-1.674408	1.233196	-0.242288
H	-3.132543	2.198161	0.073027
H	-2.780060	1.617251	-1.585993
C	0.709229	2.714553	-1.059431
C	0.834122	2.691160	-2.492711
C	0.705873	3.909062	-3.181872
H	0.791460	3.921929	-4.274987
C	0.457114	5.113418	-2.516844
H	0.339680	6.048326	-3.084730
C	0.372022	5.117444	-1.126816
H	0.184861	6.071661	-0.614673
C	0.520556	3.945983	-0.353929
C	1.071714	1.391367	-3.296760
C	2.329222	0.652745	-2.789131
H	2.494818	-0.275862	-3.372705
H	2.253161	0.372877	-1.724102
H	3.227837	1.292488	-2.903015
C	1.308939	1.674801	-4.795041
H	2.181784	2.337744	-4.959920
H	0.425272	2.131109	-5.284071
H	1.512395	0.716970	-5.314523
C	-0.181798	0.493943	-3.210233
H	-0.050482	-0.422039	-3.820469
H	-1.072954	1.031431	-3.590805
H	-0.409410	0.173156	-2.179100
C	0.420384	4.142787	1.182339
C	1.349232	5.308439	1.608544
H	2.402599	5.089591	1.340472
H	1.296300	5.446668	2.707824
H	1.076098	6.274317	1.143235
C	-1.042488	4.495304	1.541259
H	-1.389184	5.399945	1.003849
H	-1.141302	4.682867	2.630963
H	-1.722676	3.661766	1.274647
C	0.838043	2.937867	2.038680
H	0.121522	2.100065	1.955885
H	0.855200	3.240820	3.105835
H	1.847054	2.569547	1.771359
C	-0.711940	-2.634263	3.232630
H	-1.397460	-2.503439	2.372121
H	-1.325557	-2.894686	4.120027
H	-0.053867	-3.497845	3.011466
C	1.314005	-1.390597	5.166457
H	2.017565	-2.239686	5.053241
H	0.632077	-1.628708	6.009681
H	1.903143	-0.494834	5.451089
C	-0.900598	0.341747	4.037024
H	-0.343844	1.243967	4.362864
H	-1.559820	0.030562	4.874335
H	-1.551200	0.633397	3.188714
C	2.845701	-3.349320	2.195524
H	2.507979	-3.581467	3.225354
H	3.827805	-3.843318	2.044109
H	2.123178	-3.803216	1.490087
C	4.288699	-0.783565	3.135825
H	4.430207	0.305368	2.973032
H	5.274009	-1.275898	2.996842
H	3.975120	-0.931753	4.187627
C	3.770145	-1.225571	0.181407
H	3.154136	-1.676248	-0.621743
H	4.775373	-1.695749	0.135459
H	3.896619	-0.147248	-0.048388

Conformation 33.
Multiplicity: 2
Charge: 0
E(B97-3c) = -2948.797897032777 Hartree
E(M06/def2-TZVP) = -2948.911673040435 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -2947.690176946010 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -2947.965346112416 Hartree
E(PBEh-3c) = -2944.950169364931 Hartree
E(PM6) = -243.08368 Kcal/mol
E(PM7) = -239.63652 Kcal/mol
E(ωB97X-V/def2-TZVP) = -2950.749844454588 Hartree
E(GFN1-xTB) = -183.922041756334 Hartree
E(GFN2-xTB) = -119.359085331138 Hartree
E(GFN-FF) = -16.242295614269 Hartree

Coordinates:

Ti	0.441880	0.048089	0.141416
Si	3.428986	-1.540195	-0.088390
Si	3.183687	1.457676	-1.251333
O	-0.321179	1.624142	0.632865
O	-0.544562	-1.457561	-0.140713
C	2.508642	0.121297	-0.081053
H	2.649524	0.541980	0.954145
C	-1.141709	2.635909	1.003867
C	-0.999992	3.188084	2.317429
C	-1.867937	4.237536	2.671533
H	-1.795701	4.686036	3.669668
C	-2.826093	4.733668	1.783606
H	-3.489217	5.556362	2.089891
C	-2.937943	4.182947	0.504453
H	-3.695291	4.590380	-0.176046
C	-2.113321	3.126265	0.073117
C	0.059335	2.680796	3.323807
C	-0.172497	1.191387	3.660040
H	-1.193620	1.027094	4.057631
H	0.555133	0.853071	4.426508
H	-0.048517	0.537360	2.776068
C	1.477339	2.881869	2.743970
H	1.609188	2.345621	1.789169
H	2.241047	2.513130	3.459858
H	1.673411	3.956194	2.554350
C	0.000858	3.452014	4.657910
H	0.191014	4.535625	4.523927
H	0.784091	3.060481	5.337671
H	-0.974476	3.329954	5.170396
C	-2.294816	2.537673	-1.348025
C	-2.789223	1.075436	-1.260385
H	-2.066181	0.403867	-0.763489
H	-2.971143	0.668053	-2.276764
H	-3.738419	1.015012	-0.692071
C	-0.981685	2.618106	-2.158731
H	-0.620811	3.663944	-2.226697
H	-1.144957	2.243432	-3.190334
H	-0.171837	2.013961	-1.709460
C	-3.354847	3.316321	-2.154365
H	-4.358566	3.264554	-1.687765
H	-3.438737	2.871800	-3.166193
H	-3.082375	4.383269	-2.280007
C	-1.309348	-2.548730	-0.363288
C	-2.095455	-3.071308	0.719875
C	-2.830280	-4.244603	0.481022
H	-3.434807	-4.677706	1.286889
C	-2.815131	-4.885587	-0.762895
H	-3.392684	-5.808999	-0.917437
C	-2.071810	-4.337853	-1.806548
H	-2.078126	-4.845435	-2.781818
C	-1.312816	-3.157700	-1.654836
C	-2.158759	-2.387243	2.105867
C	-0.762204	-2.362113	2.766257
H	-0.819883	-1.900156	3.772883
H	-0.030660	-1.782695	2.171812
H	-0.363590	-3.390235	2.878041
C	-3.091280	-3.144260	3.074506
H	-2.746179	-4.180020	3.265239
H	-4.134622	-3.186138	2.702880
H	-3.107063	-2.615343	4.048377
C	-2.730344	-0.956777	1.969412
H	-2.842287	-0.490845	2.969318
H	-3.728652	-0.981038	1.488696
H	-2.085309	-0.292883	1.367743
C	-0.555071	-2.671358	-2.920079
C	0.155655	-1.308854	-2.824629
H	-0.543073	-0.489025	-2.569980
H	0.597950	-1.067158	-3.812323
H	0.989997	-1.310857	-2.098555
C	0.514600	-3.729398	-3.282249
H	1.244999	-3.850645	-2.457254
H	1.072099	-3.422826	-4.191881
H	0.064419	-4.721992	-3.479094
C	-1.567512	-2.538438	-4.085123
H	-2.078384	-3.491786	-4.318021
H	-1.045435	-2.205411	-5.005650
H	-2.347128	-1.788207	-3.841515
C	3.959452	-2.059147	-1.836411
H	3.091351	-2.155250	-2.517969
H	4.455948	-3.050345	-1.787155
H	4.674254	-1.346488	-2.293068
C	4.968422	-1.408041	1.015545
H	5.665158	-0.623162	0.661177
H	5.517389	-2.372450	1.041367
H	4.676443	-1.158857	2.057047
C	2.384847	-2.963456	0.616050
H	2.061722	-2.755816	1.656491
H	2.996272	-3.890148	0.637381
H	1.475197	-3.170573	0.017880
C	2.598041	3.187905	-0.735255
H	1.497289	3.265971	-0.645706
H	2.934201	3.927025	-1.492281
H	3.038527	3.483354	0.238139
C	2.641027	1.164395	-3.045736
H	2.936446	0.163095	-3.414454
H	3.115199	1.923267	-3.702529
H	1.542961	1.259456	-3.159978
C	5.085666	1.538263	-1.222823

H	5.456895	1.751252	-0.199329
H	5.431849	2.359329	-1.885127
H	5.564993	0.601290	-1.569341

Conformation 34.
Multiplicity: 2
Charge: 0
E(B97-3c) = -2948.793606837194 Hartree
E(M06/def2-TZVP) = -2948.907717400867 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -2947.685639913320 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -2947.961066829451 Hartree
E(PBEh-3c) = -2944.946018581296 Hartree
E(PM6) = -241.79341 Kcal/mol
E(PM7) = -238.47640 Kcal/mol
E(ωB97X-V/def2-TZVP) = -2949.533379306207 Hartree
E(GFN1-xTB) = -184.321434540650 Hartree
E(GFN2-xTB) = -119.355282959582 Hartree
E(GFN-FF) = -16.239270560723 Hartree

Coordinates:

Ti	-0.020270	0.524757	-0.014373
Si	2.279271	2.881064	-0.542367
Si	-0.516942	3.154804	-2.145403
O	0.727286	-0.069710	1.534704
O	-1.057999	-0.566998	-1.025009
C	0.436812	2.451505	-0.665384
H	-0.038745	2.923543	0.239274
C	1.102536	-0.684409	2.678865
C	1.928937	-1.856255	2.592700
C	2.310140	-2.471585	3.797020
H	2.942728	-3.367069	3.770844
C	1.902291	-1.976195	5.040617
H	2.215032	-2.479909	5.967279
C	1.098026	-0.839403	5.095099
H	0.786335	-0.460744	6.079457
C	0.674419	-0.156906	3.934797
C	2.387443	-2.454175	1.241307
C	3.326258	-3.661941	1.441444
H	4.245689	-3.388646	1.997082
H	3.638564	-4.045641	0.449579
H	2.830167	-4.496217	1.976371
C	1.165359	-2.968548	0.445928
H	0.614819	-3.735869	1.025962
H	1.494456	-3.432963	-0.506934
H	0.445224	-2.170087	0.192610
C	3.181372	-1.413950	0.419050
H	2.568968	-0.535212	0.147095
H	3.550241	-1.869780	-0.522901
H	4.058264	-1.047063	0.989452
C	-0.205982	1.099506	4.175453
C	-0.693362	1.858341	2.926930
H	0.149290	2.246661	2.326640
H	-1.298523	2.729354	3.253517
H	-1.345623	1.236507	2.280569
C	0.616554	2.113576	5.009135
H	0.945285	1.691972	5.978532
H	0.010571	3.018638	5.222204
H	1.523054	2.427370	4.452882
C	-1.470781	0.678437	4.962007
H	-2.073242	-0.045548	4.376135
H	-2.105066	1.565020	5.169444
H	-1.227242	0.204982	5.932600
C	-1.808182	-1.502190	-1.645082
C	-1.397006	-2.000756	-2.918016
C	-2.261993	-2.915697	-3.554783
H	-1.993420	-3.300233	-4.549059
C	-3.450387	-3.348800	-2.968612
H	-4.100759	-4.062332	-3.496058
C	-3.807376	-2.876643	-1.700196
H	-4.738041	-3.240395	-1.248184
C	-3.010443	-1.952831	-1.002829
C	-0.108965	-1.615480	-3.696795
C	0.947048	-0.799249	-2.924686
H	1.842751	-0.675609	-3.567400
H	1.274689	-1.311298	-2.000113
H	0.595822	0.216252	-2.667226
C	-0.522798	-0.793034	-4.940528
H	-1.025847	0.148427	-4.641717
H	-1.220767	-1.355113	-5.592196
H	0.370053	-0.526789	-5.544187
C	0.611200	-2.910038	-4.150075
H	1.532821	-2.651624	-4.710902
H	-0.010424	-3.542755	-4.811744
H	0.903950	-3.522938	-3.273308
C	-3.436775	-1.465420	0.404292
C	-2.377335	-1.863940	1.458322
H	-2.204690	-2.958494	1.449773
H	-2.723618	-1.581494	2.474247
H	-1.400950	-1.372948	1.298167
C	-3.665893	0.063730	0.419257
H	-2.739224	0.632125	0.207033
H	-4.034875	0.383943	1.415647
H	-4.419528	0.357518	-0.338640
C	-4.765196	-2.113024	0.848174
H	-5.603784	-1.855377	0.170868
H	-5.028203	-1.743156	1.859270
H	-4.691013	-3.217218	0.908071
C	2.909542	2.568401	1.223824
H	2.383454	3.223406	1.949643
H	3.992094	2.804652	1.288200
H	2.766264	1.519776	1.549908
C	3.317663	1.859221	-1.757976
H	3.243664	0.772884	-1.553094
H	4.386384	2.147408	-1.674810
H	3.001353	2.028141	-2.806066
C	2.610865	4.719834	-0.902847
H	2.345867	4.999703	-1.942355
H	3.687721	4.947281	-0.756627
H	2.030632	5.371269	-0.217456
C	-2.154366	2.240781	-2.451978
H	-2.005910	1.166044	-2.674617
H	-2.683997	2.702265	-3.311722
H	-2.826789	2.308164	-1.572098
C	0.487665	3.076762	-3.754793
H	1.412070	3.686040	-3.700737
H	-0.127172	3.472415	-4.589660
H	0.777764	2.039677	-4.015164
C	-0.970221	4.968206	-1.804275
H	-1.588349	5.051866	-0.886002
H	-1.559116	5.389486	-2.645788
H	-0.069538	5.597982	-1.664513

Conformation 9.
Multiplicity: 2
Charge: 0
E(B97-3c) = -2948.804852850955 Hartree
E(M06/def2-TZVP) = -2948.916764770754 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -2947.696434917210 Hartree
E(PBE0 - D3(BJ)/def2-TZVP) = -2947.970999992164 Hartree
E(PBEh-3c) = -2944.954722030579 Hartree
E(PM6) = -242.88212 Kcal/mol
E(PM7) = -240.24007 Kcal/mol
E(ωB97X-V/def2-TZVP) = -2950.753886133855 Hartree
E(GFN1-xTB) = -184.676767207757 Hartree
E(GFN2-xTB) = -119.364870949251 Hartree
E(GFN-FF) = -16.241107833530 Hartree

Coordinates:

Ti	0.382302	-0.113896	-0.234362
Si	2.987610	1.634351	-1.694703
Si	3.058992	-1.578517	-1.310113
O	0.367039	0.892064	1.289678
O	-1.039142	-1.040786	-0.926181
C	2.034670	0.013480	-1.484187
H	1.476937	-0.132437	-2.442613
C	-0.071879	1.407400	2.466064
C	0.432396	0.860267	3.689451
C	-0.096499	1.369013	4.890545
H	0.256381	0.968741	5.848887
C	-1.063552	2.377630	4.902033
H	-1.462178	2.750019	5.857497
C	-1.508108	2.924466	3.695563
H	-2.250609	3.731121	3.726755
C	-1.029603	2.471459	2.451423
C	1.522435	-0.235938	3.726734
C	1.967257	-0.553408	5.169171
H	2.379299	0.338116	5.682885
H	2.765355	-1.322020	5.140567
H	1.140483	-0.959925	5.785385
C	0.990895	-1.555139	3.125040
H	0.112349	-1.922573	3.691225
H	1.775964	-2.339024	3.155438
H	0.678962	-1.440371	2.068359
C	2.778819	0.236089	2.962570
H	2.570327	0.414701	1.893945
H	3.579805	-0.527974	3.039286
H	3.168657	1.181858	3.389813
C	-1.521291	3.138483	1.145289
C	-2.437118	4.346983	1.429773
H	-3.370344	4.055242	1.951847
H	-2.730857	4.812641	0.467774
H	-1.926431	5.122793	2.034518
C	-2.350979	2.150623	0.295480
H	-1.780896	1.254224	-0.014595
H	-2.704330	2.643606	-0.633206
H	-3.236758	1.794782	0.856966
C	-0.317200	3.673658	0.339425
H	0.253561	4.416901	0.931973
H	-0.668157	4.171346	-0.588012
H	0.380652	2.868308	0.050678
C	-2.272237	-1.422531	-1.344171
C	-2.652004	-1.153829	-2.699890

C	-3.956503	-1.504432	-3.093263
H	-4.285266	-1.300278	-4.119743
C	-4.851990	-2.113449	-2.210610
H	-5.867614	-2.373201	-2.544818
C	-4.445958	-2.406818	-0.906318
H	-5.156927	-2.905107	-0.236142
C	-3.159994	-2.082858	-0.433216
C	-1.679008	-0.523913	-3.720346
C	-0.439587	-1.437769	-3.876870
H	0.310714	-0.966423	-4.545625
H	-0.734652	-2.407269	-4.326320
H	0.044991	-1.653820	-2.909132
C	-1.287729	0.907978	-3.289493
H	-0.774481	0.943340	-2.308338
H	-2.189644	1.547656	-3.209686
H	-0.605768	1.365882	-4.034767
C	-2.311363	-0.395523	-5.121387
H	-1.562882	0.032180	-5.818368
H	-3.191002	0.279101	-5.125396
H	-2.623087	-1.377470	-5.529976
C	-2.757217	-2.458292	1.011649
C	-1.511649	-3.372685	0.989974
H	-1.727883	-4.310173	0.438816
H	-1.213518	-3.643332	2.023631
H	-0.648340	-2.887993	0.502008
C	-2.494666	-1.186927	1.847176
H	-1.652590	-0.589963	1.459406
H	-2.253108	-1.452802	2.896080
H	-3.387825	-0.531590	1.858366
C	-3.872868	-3.239462	1.735487
H	-4.798249	-2.639953	1.848713
H	-3.525103	-3.504377	2.754046
H	-4.129172	-4.183169	1.213748
C	4.549927	1.435501	-2.765151
H	5.292927	0.743681	-2.320528
H	5.043747	2.422007	-2.890772
H	4.294569	1.056489	-3.775970
C	1.893515	2.873658	-2.629084
H	1.671173	2.496583	-3.648856
H	2.418103	3.845838	-2.737079
H	0.928743	3.062564	-2.120321
C	3.524037	2.368415	-0.032363
H	2.658529	2.574558	0.627820
H	4.066692	3.322274	-0.197254
H	4.205428	1.680672	0.507692
C	3.662818	-2.134784	-3.021398
H	2.802393	-2.308053	-3.700549
H	4.231306	-3.085096	-2.943571
H	4.320608	-1.376409	-3.489442
C	2.032415	-3.025966	-0.612431
H	1.746603	-2.870203	0.448290
H	2.639986	-3.955403	-0.653370
H	1.105801	-3.211034	-1.193724
C	4.536826	-1.345389	-0.147734
H	5.238827	-0.568848	-0.510935
H	5.101194	-2.296807	-0.059810
H	4.202797	-1.053336	0.867246